Spectroscopy: A thousand pictures

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with many thanks to many collaborators

MIPSE seminar

March 6, 2024

SAND2024-02586PE

Context: we are interested in matter at extreme conditions relevant to fusion and astrophysical plasmas

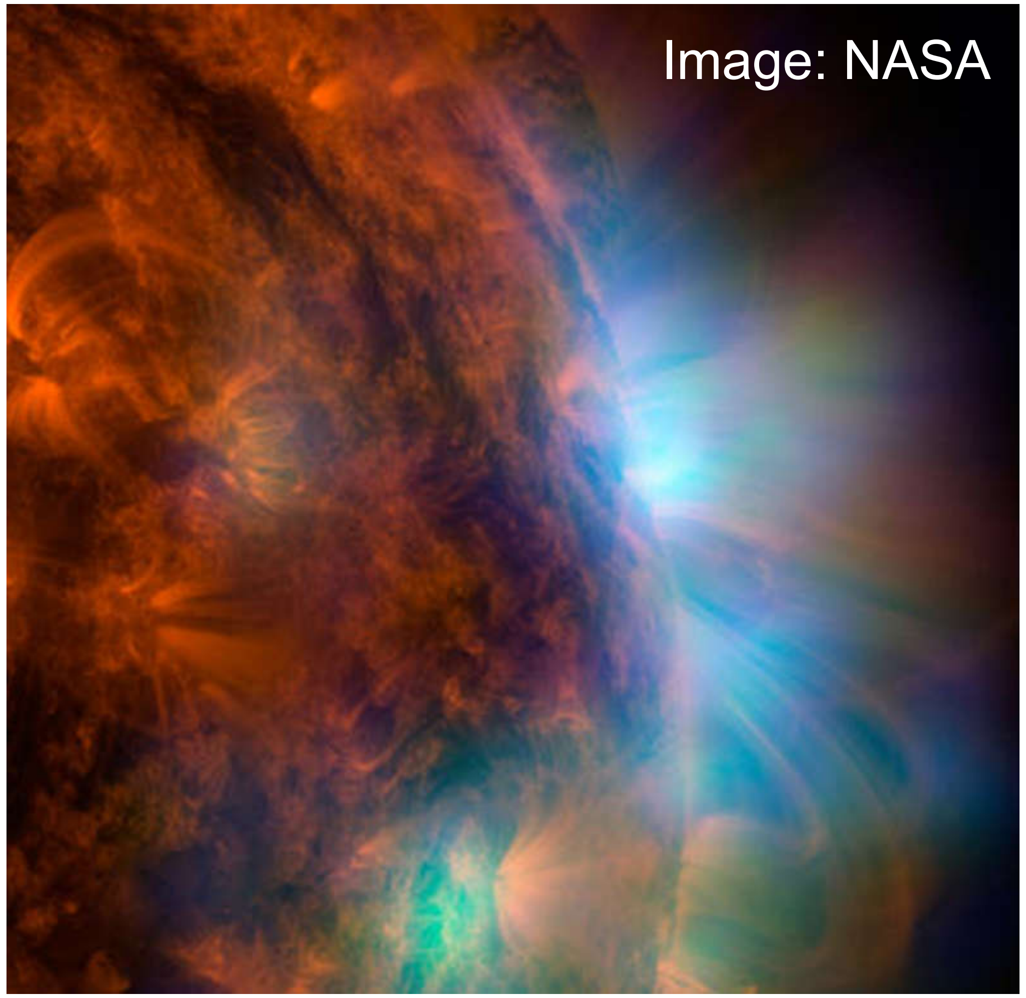
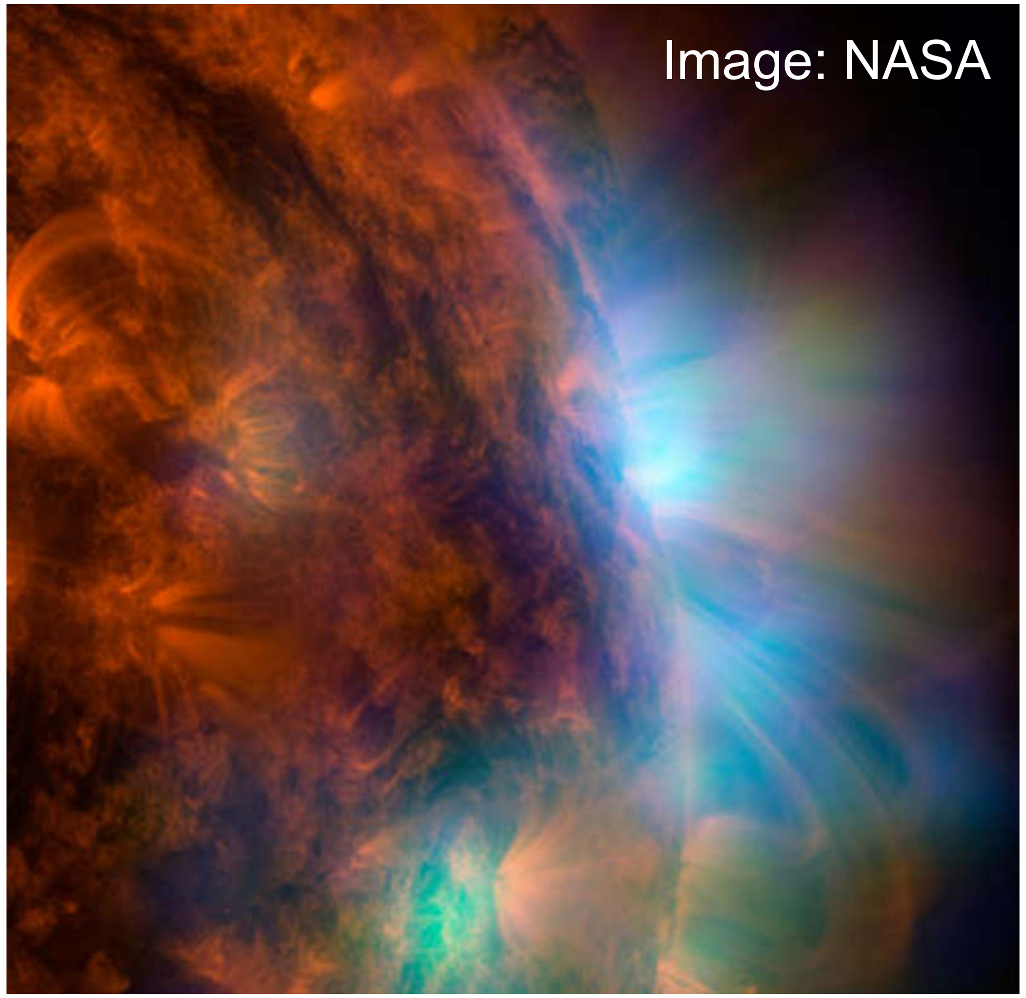


Image: NASA

10^{+9} meters
10^{+17} seconds

Context: we are interested in matter at extreme conditions relevant to fusion and astrophysical plasmas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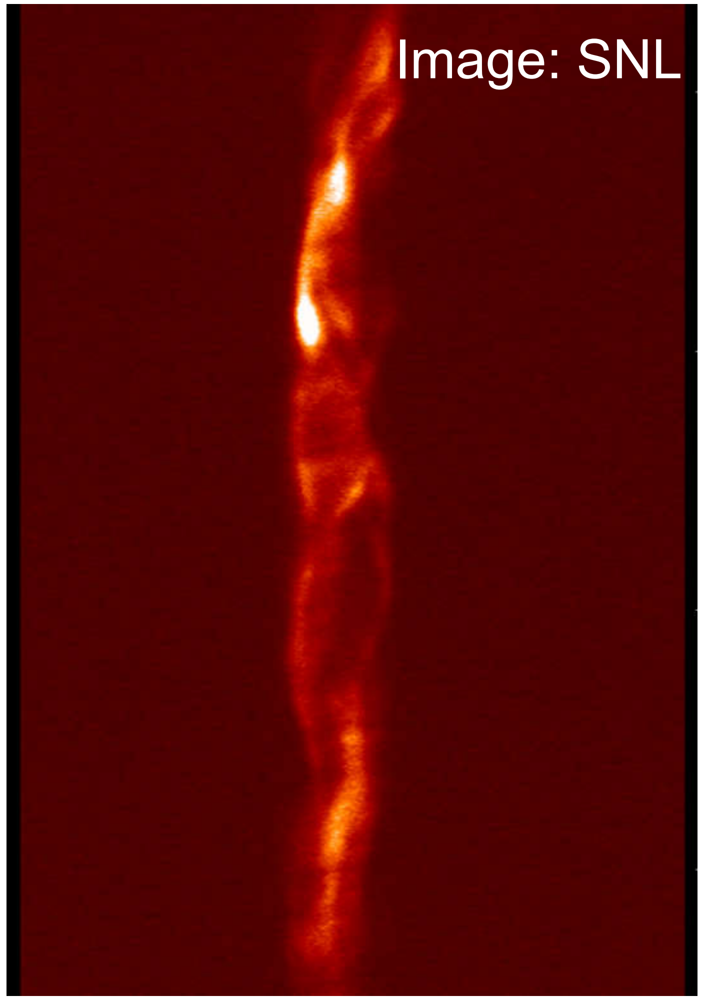
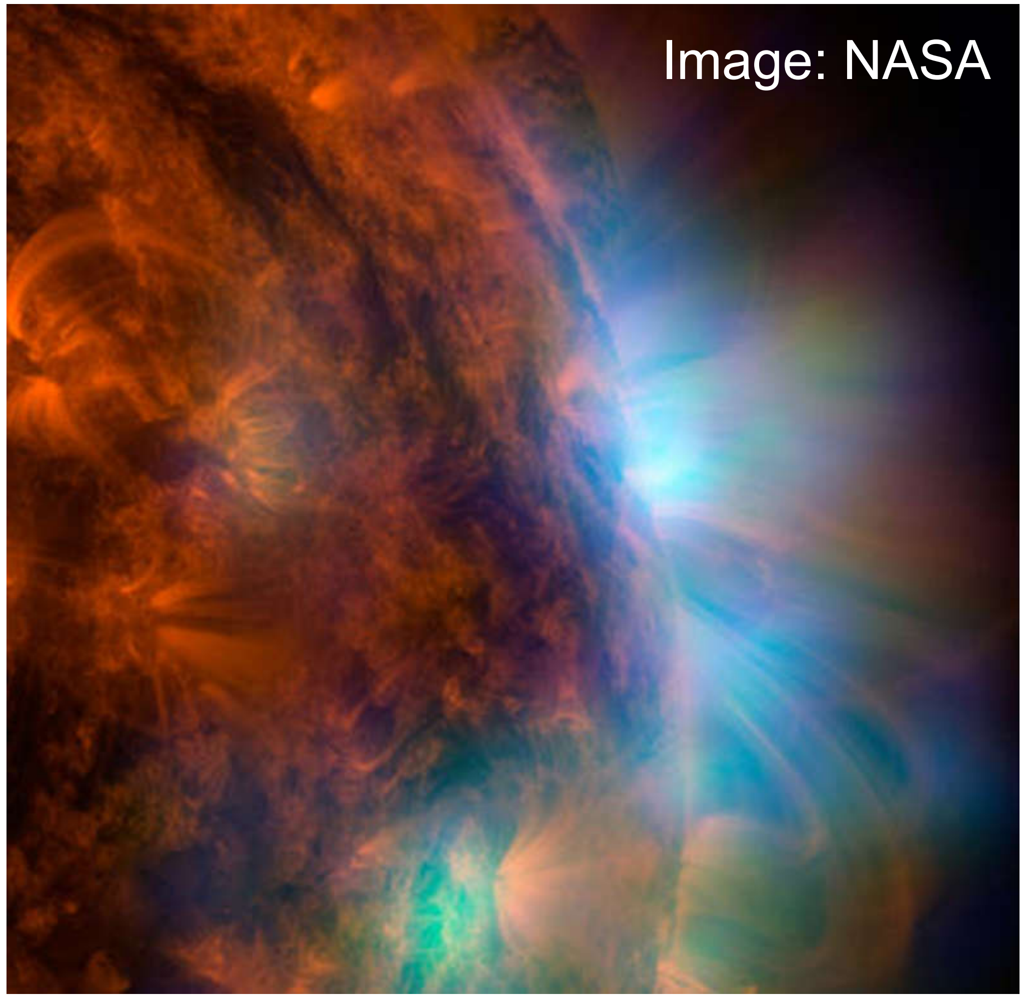


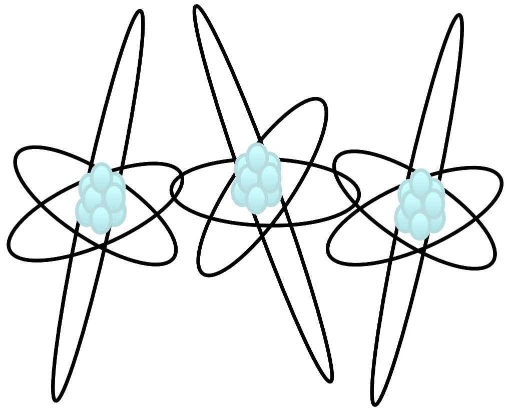
Image: SNL

10^{-4} meters
10^{-9} seconds

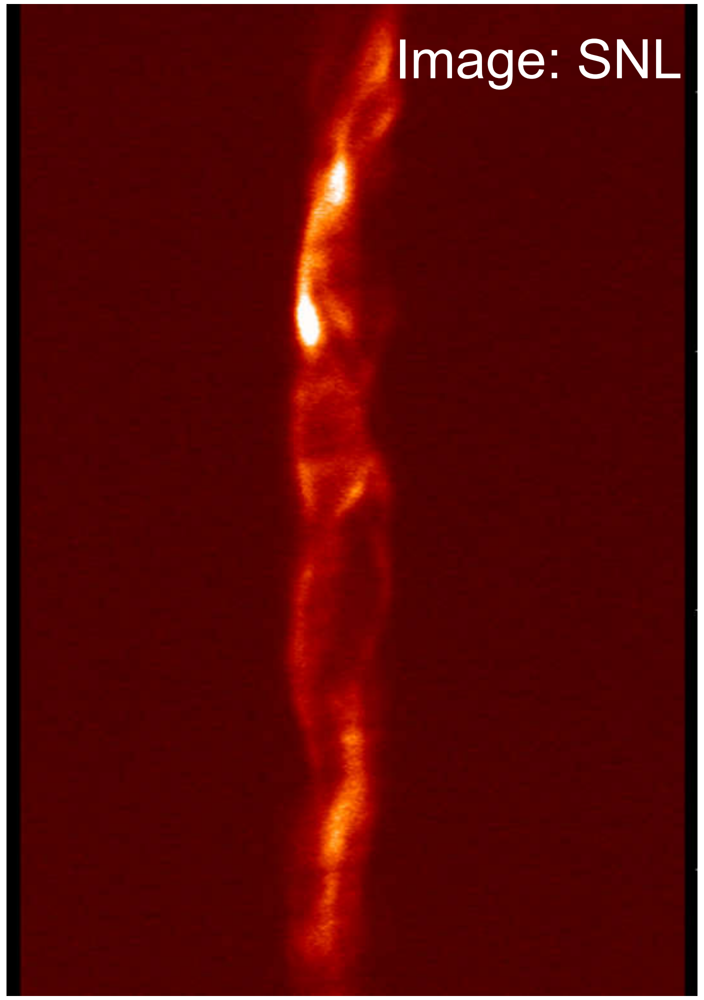
Context: we are interested in matter at extreme conditions relevant to fusion and astrophysical plasmas



10^{+9} meters
10^{+17} seconds



10^{-10} meters
10^{-14} seconds

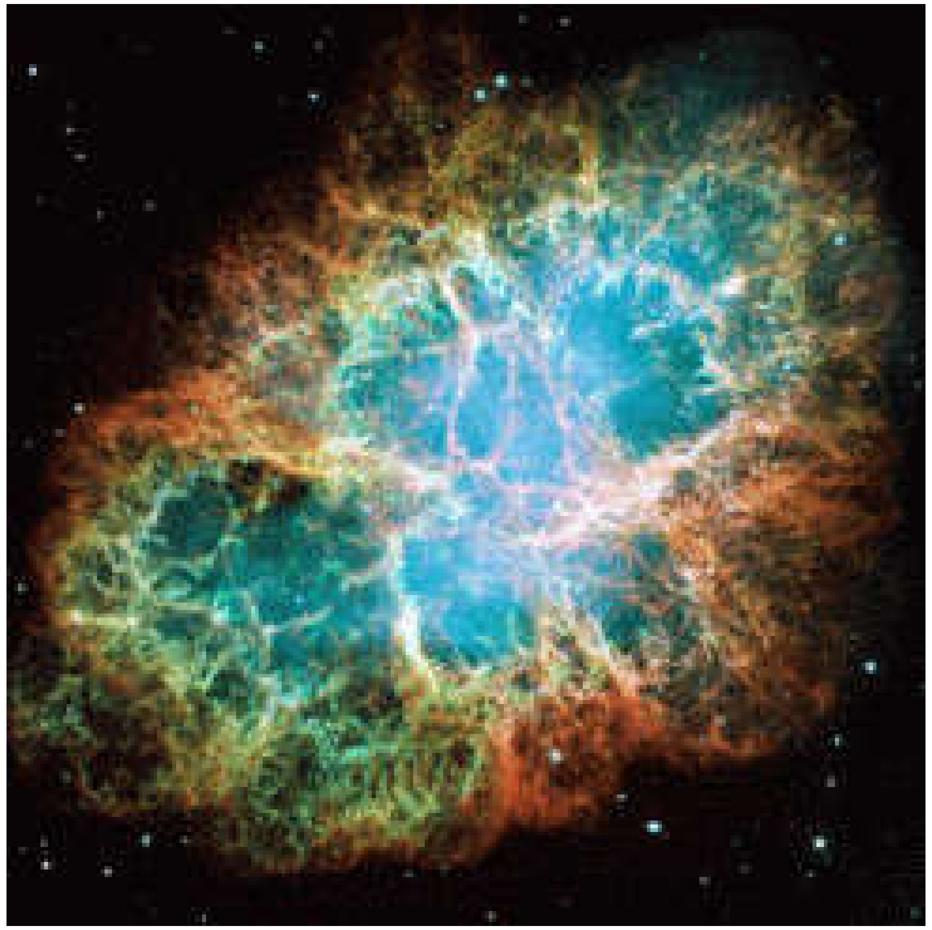


10^{-4} meters
10^{-9} seconds

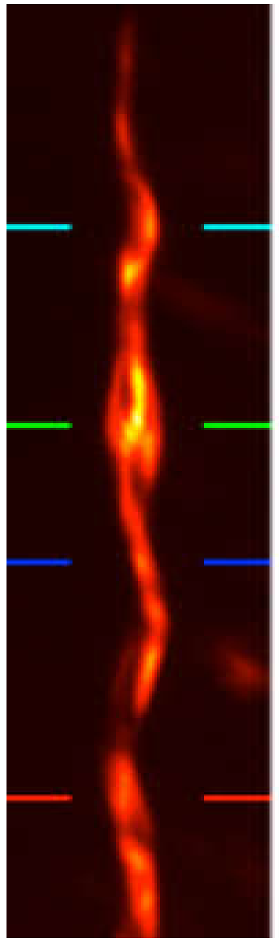
Understanding atomic properties plays a critical role in modeling and understanding larger plasma systems

At the object scale, we have two basic techniques to learn about HED plasmas:

1. Look at them

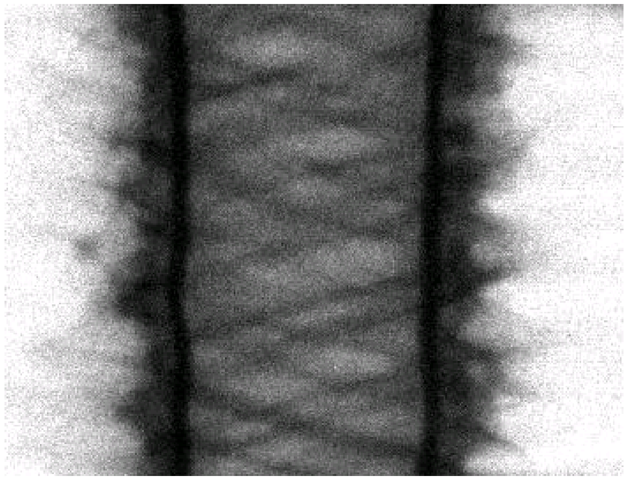


Optical image of the
Crab nebula
(HST)



X-ray image
of MagLIF
(E. Harding, SNL)

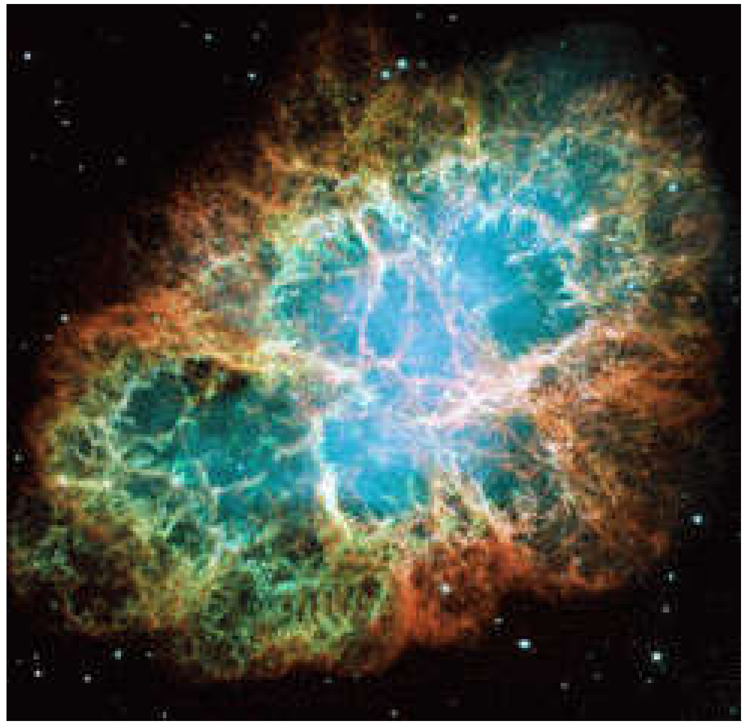
2. Hit them with something

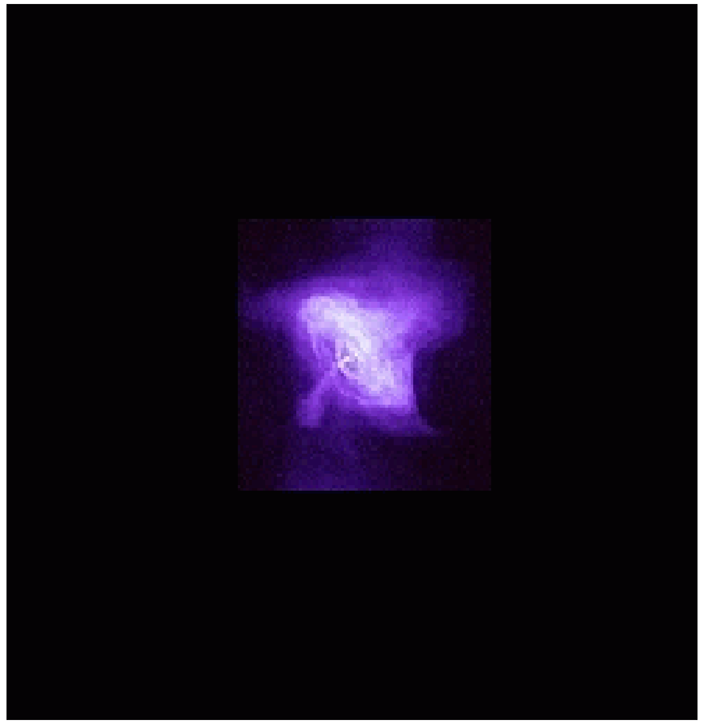


X-ray
radiography
(T. Awe, SNL)

What we see depends on how we look

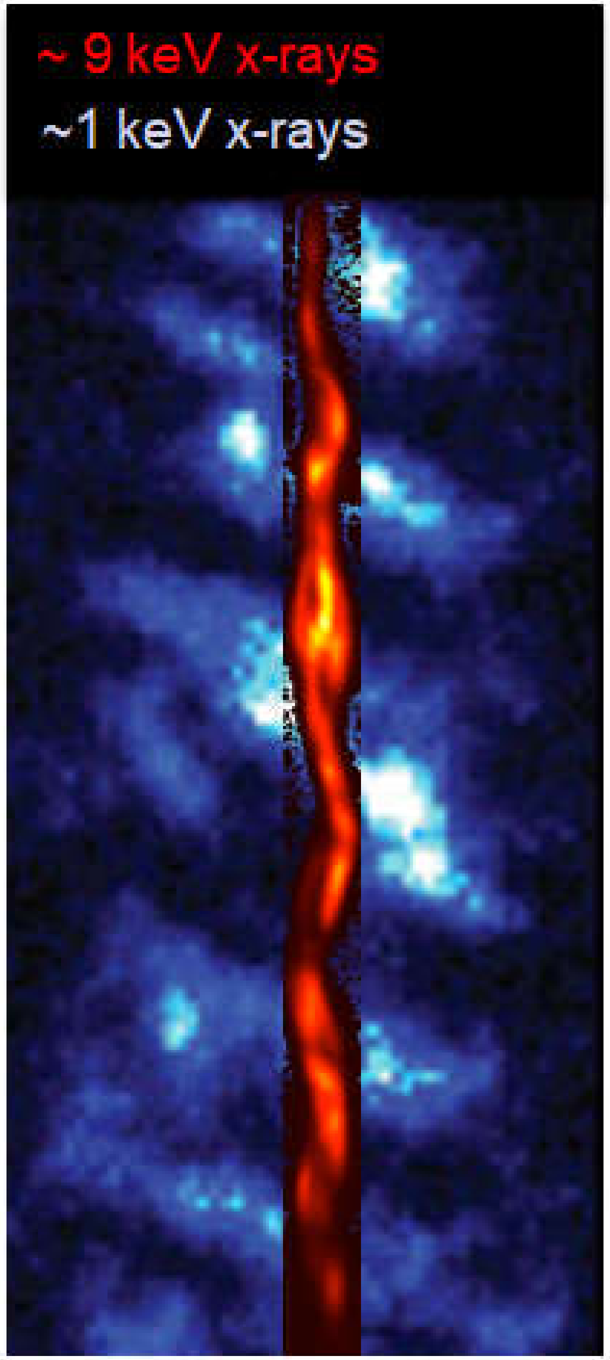
Images collected in different ways can reveal gradients and internal structure





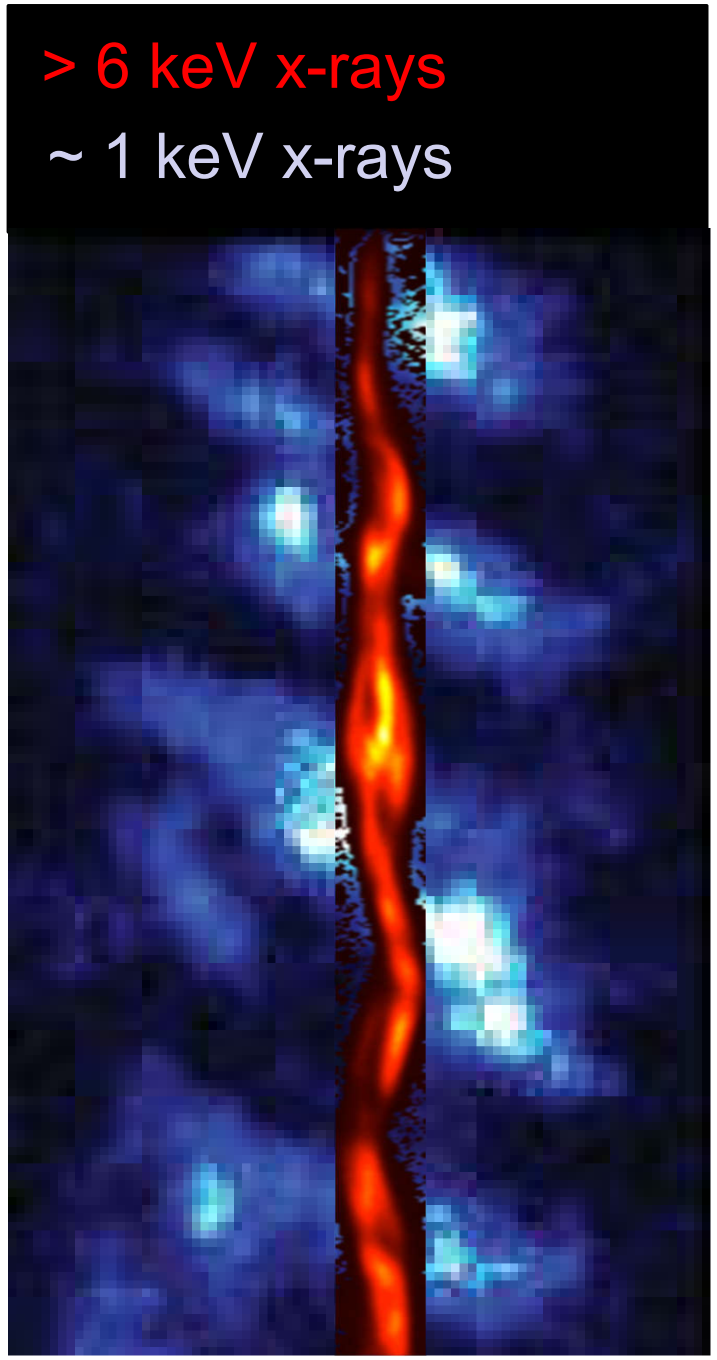
Optical

X-ray



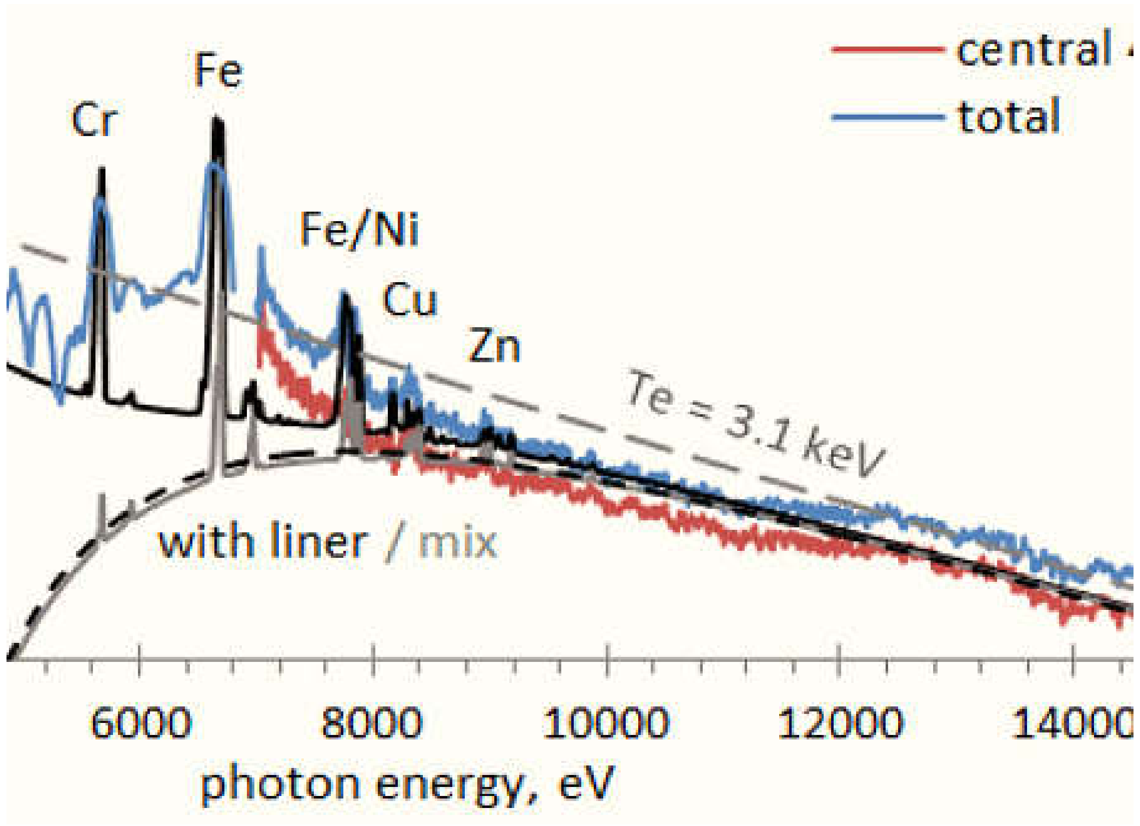
Gomez *et al* PRL 2014

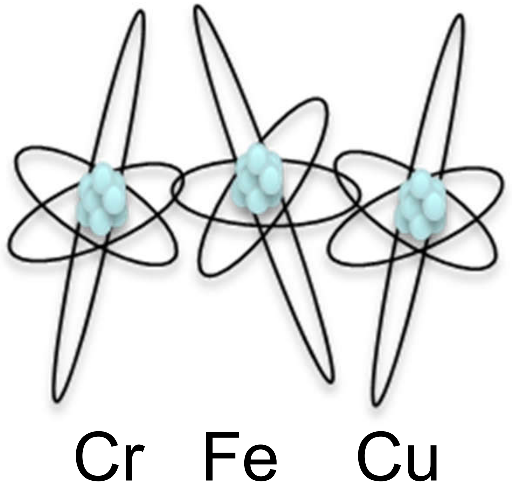
Beyond imaging, energy-resolved data can reveal details of object composition, conditions, and motion



A spectrum is worth a thousand pictures

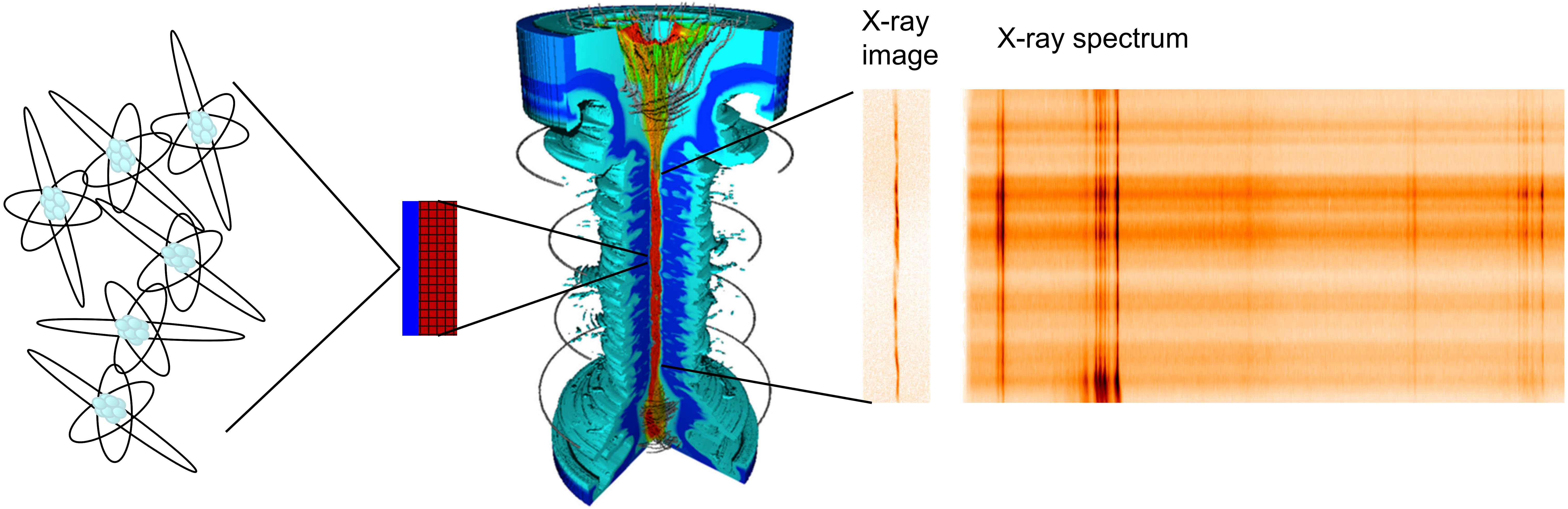
Interpreting energy-dependent data requires understanding atomic-scale structure and response





embedded in hot plasma

X-ray spectroscopy couples atomic physics and quantum mechanics with fusion and astrophysics



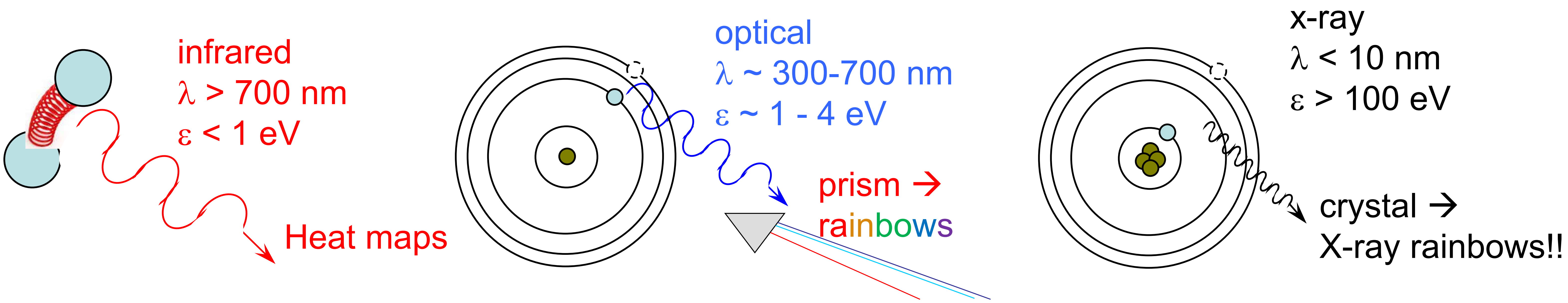
If we understand the atomic-scale response of materials in extreme conditions,

then we can more reliably simulate object-scale high energy density plasmas…

…and we can more rigorously interpret experimental and observational data

Simulation courtesy C. Jennings, Spectrum courtesy E. Harding

Spectroscopy is the science of measuring and interpreting the photons emitted and absorbed by molecules, atoms, and ions



infrared
$\lambda > 700$ nm
$\varepsilon < 1$ eV

Heat maps

optical
$\lambda \sim 300\text{-}700$ nm
$\varepsilon \sim 1 - 4$ eV

prism →
rainbows

x-ray
$\lambda < 10$ nm
$\varepsilon > 100$ eV

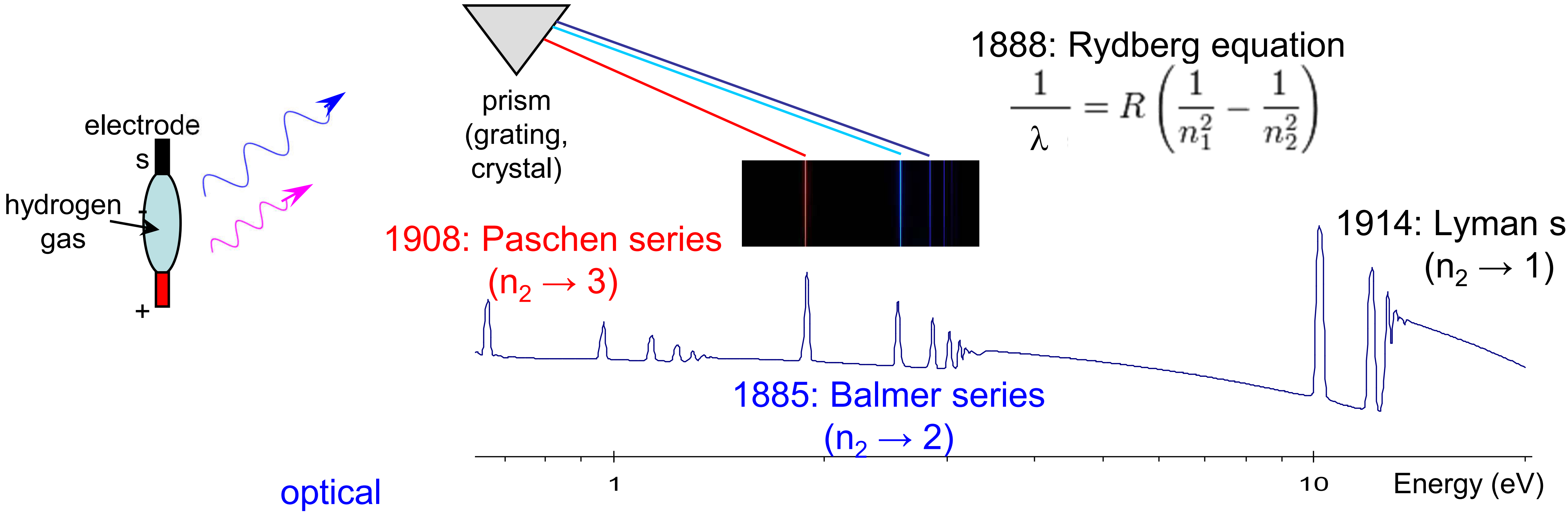
crystal →
X-ray rainbows!!

The history of spectroscopy is intricately linked to the history of modern physics

- **atomic physics and quantum mechanics**
  much of what we know about matter was learned through spectroscopy
- **astrophysics and cosmology**
  "spectroscopy puts the 'physics' in astrophysics!"
- **plasma physics and fusion research**
  spectroscopic diagnostics reveal details of temperature, density, fields…

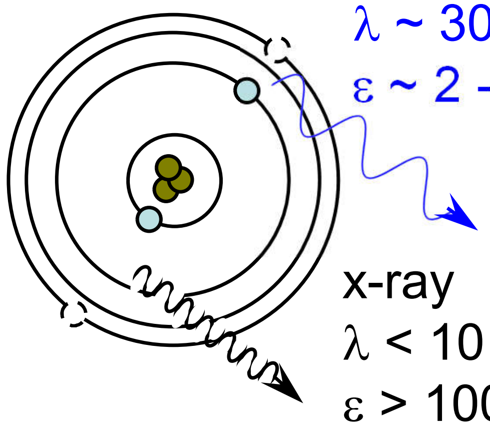
A bit of history: the first energy-resolved measurements of simple atoms revealed surprising internal structure

Around 1900, we knew that atoms were composed of heavy nuclei + light electrons (Rutherford). Regularity in the chemical behavior of different elements and intriguing patterns in the emission spectra of pure materials had been observed but not explained.



1888: Rydberg equation

$$\frac{1}{\lambda} = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$



In 1913, Neils Bohr proposed an *empirical* model of the atom that would account for the measured spectrum of hydrogen: electrons occupy discrete, stable orbitals with energies $E_n \sim (Z/n)^2$

These energy-resolved measurements were integral to the development of modern quantum theory

In 1925, Erwin Schrödinger formulated an equation to described the discrete “stationary states” of a quantum particle interacting with a potential

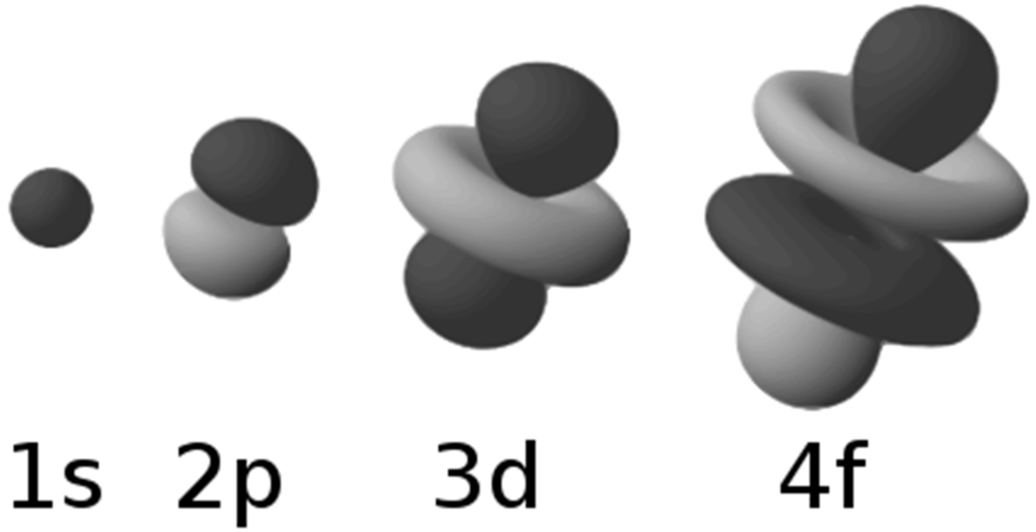
Energy eigenvalue

Potential energy ~ $-Z^2/r$

$$E\Psi(\mathbf{r}) = \frac{-\hbar^2}{2m}\nabla^2\Psi(\mathbf{r}) + V(\mathbf{r})\Psi(\mathbf{r})$$

Kinetic energy: $-p^2/2m - L^2/2mr^2$

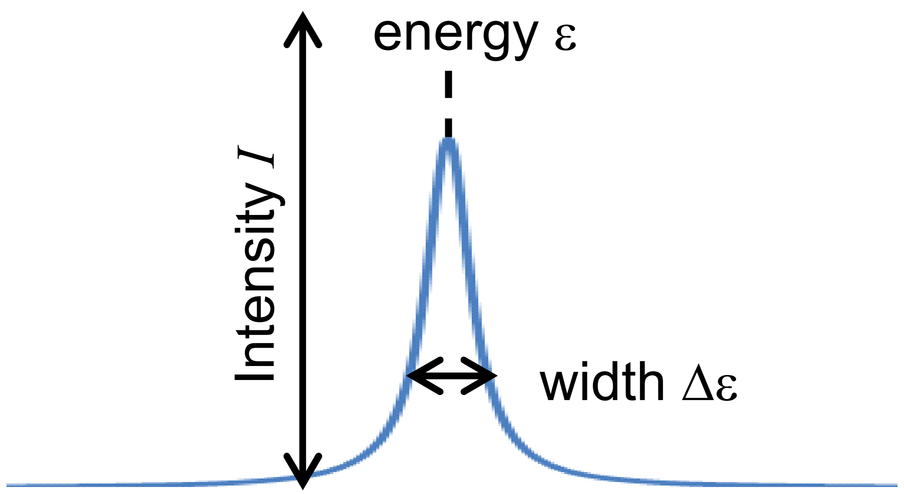
For a one-electron atom, Schrödinger’s equation can be solved analytically, giving eigenvalues that match Bohr’s empirical formula and wavefunctions that represent electronic probability distributions

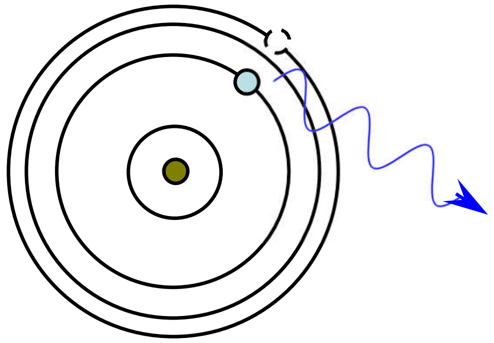


Higher precision measurements and increasingly sophisticated theory developed in tandem throughout the 1900s

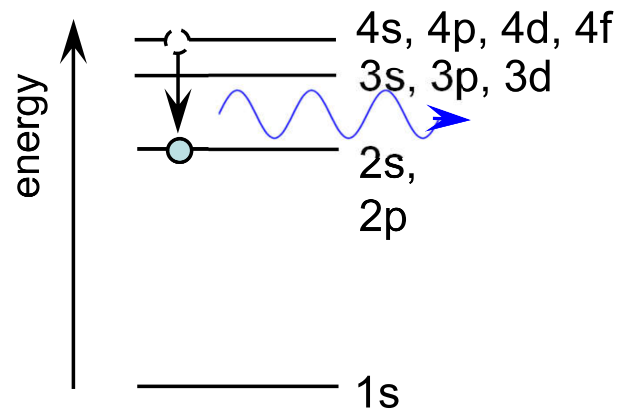
Modern theory provides exquisitely accurate predictions for the structure and spectra of isolated, one-electron ions in LTE

A single emission line can be characterized by three quantities, all of which can be derived from QM and Local Thermodynamic Equilibrium (LTE) statistics





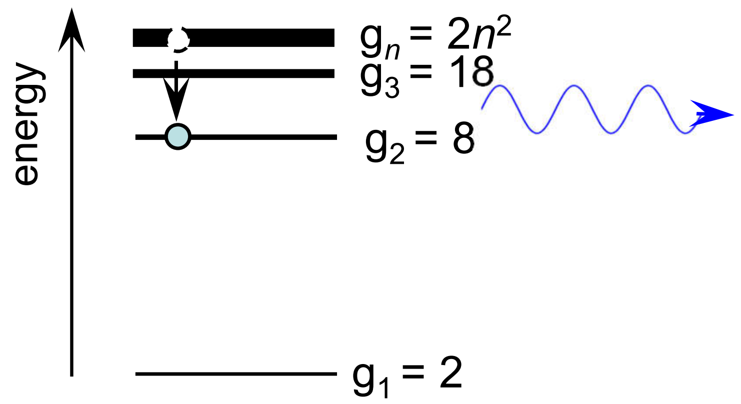
Bohr: ~ ε



Schrödinger: ~ ε and ~ A^{rad}

$A^{rad} = <\Psi_{n1} | r | \Psi_{n2}> = 1/\Delta\tau$

Heisenberg: $\Delta\varepsilon\, \Delta\tau \sim \frac{1}{2}\hbar$

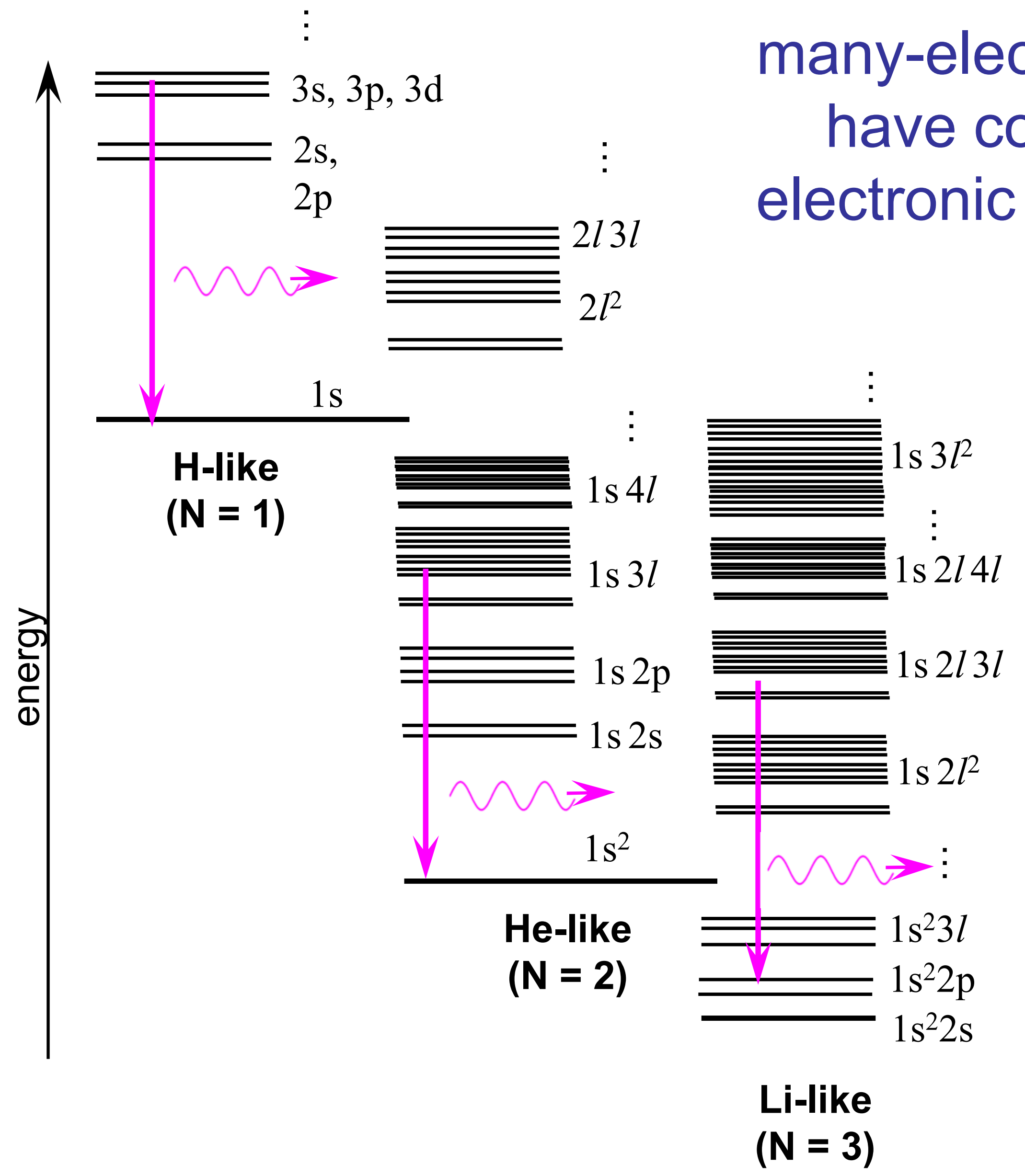


Boltzmann: $X_n = g_n e^{-\Delta E/T}$

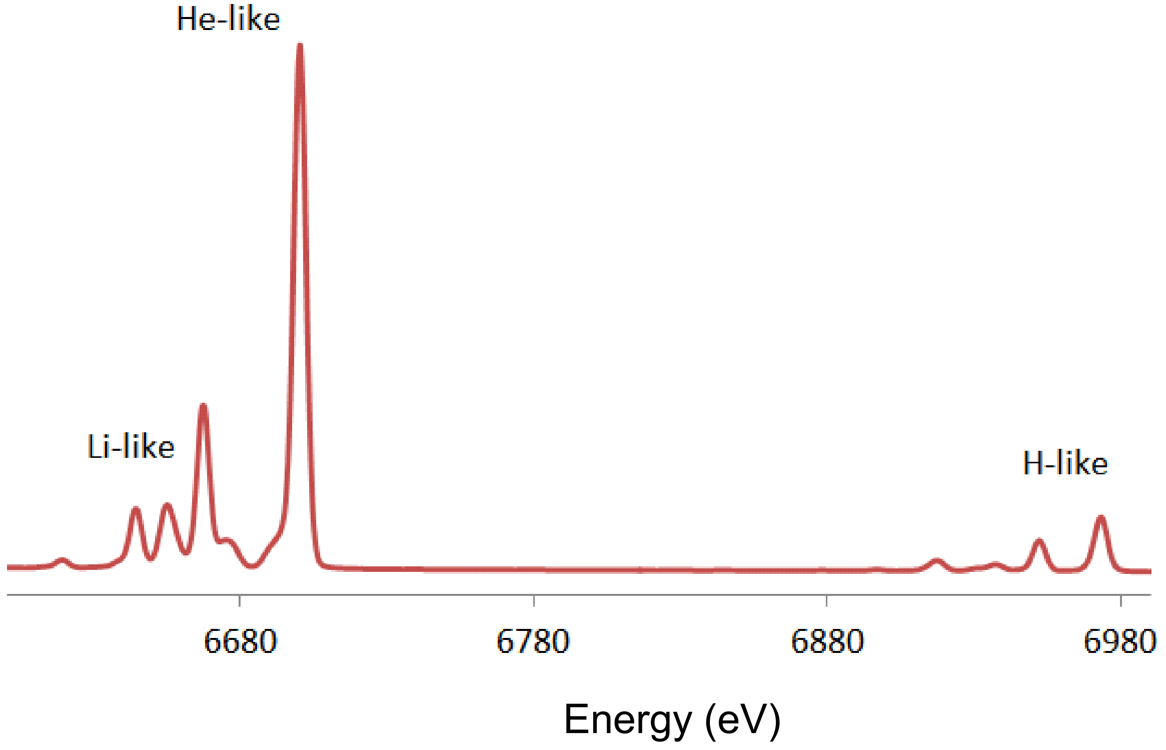
$\rightarrow I = X_n A^{rad}$

Unfortunately, not all ions are hydrogenic…

many-electron ions have complex electronic structure



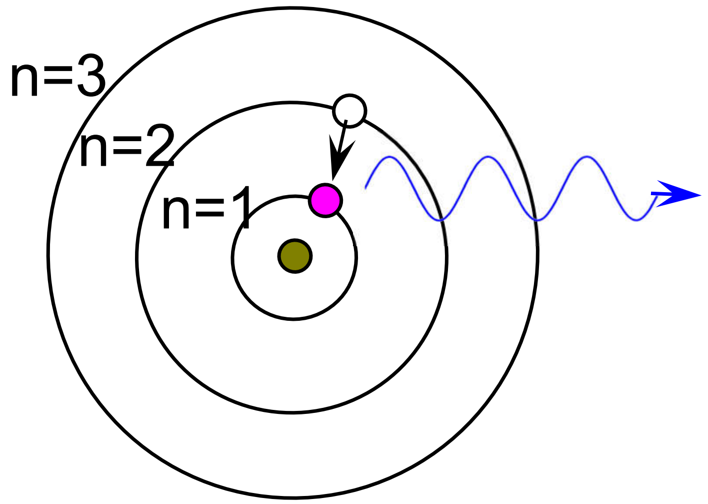
This structure is reflected in their emission spectra:

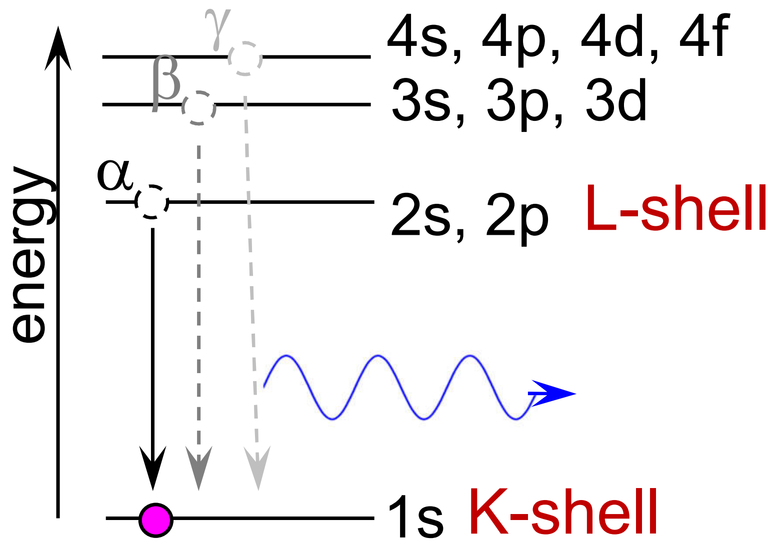


Each ion of each element has a spectroscopic "fingerprint"

Bohr model:

$\varepsilon_n \sim 13.6\ \text{eV}\ (Z/n)^2$





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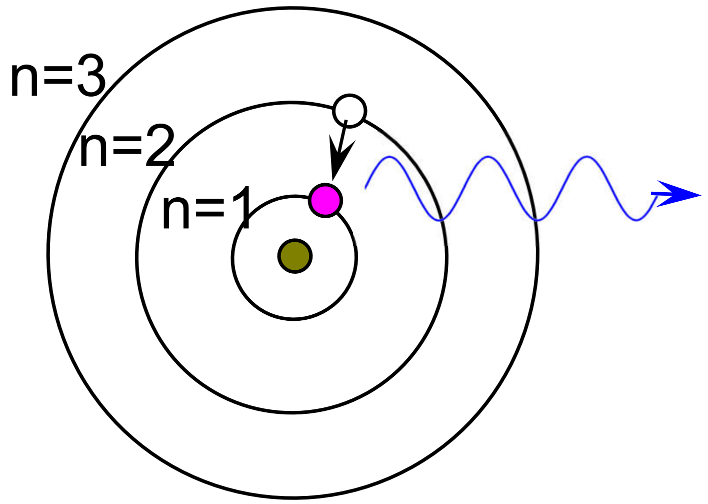
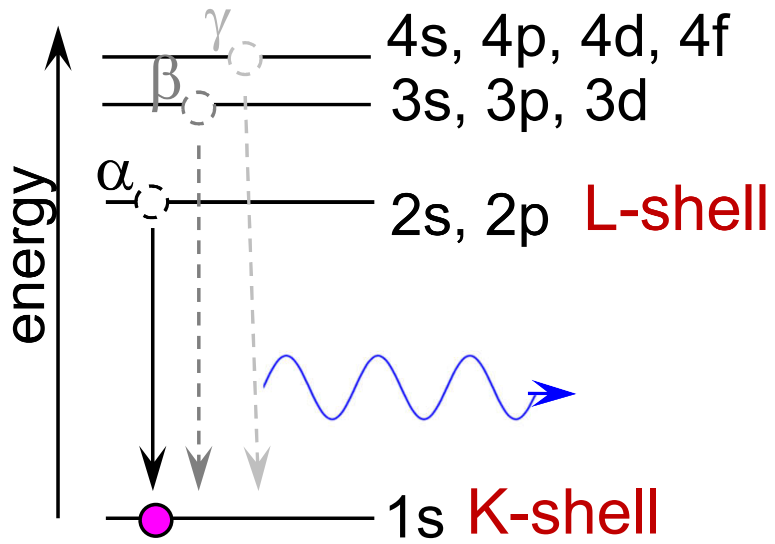
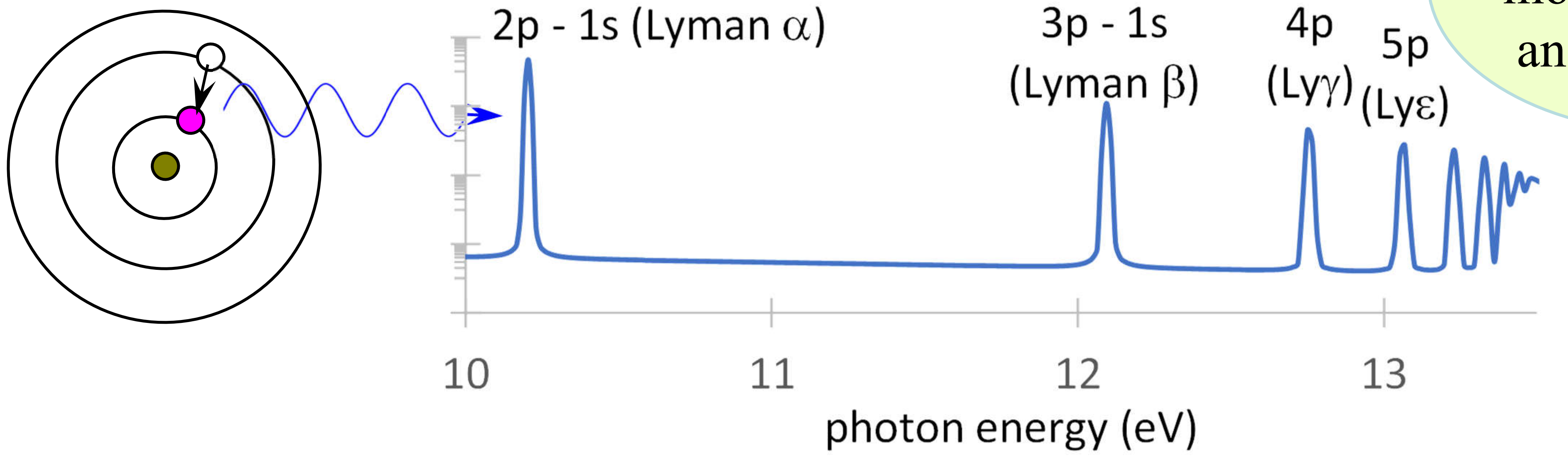


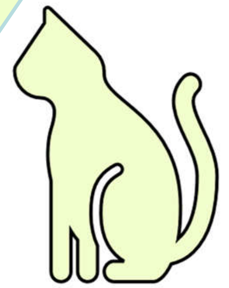


neutral hydrogen (Z = 1, n = 1)

K-shell $h\nu = \Delta\varepsilon \sim 10$ eV



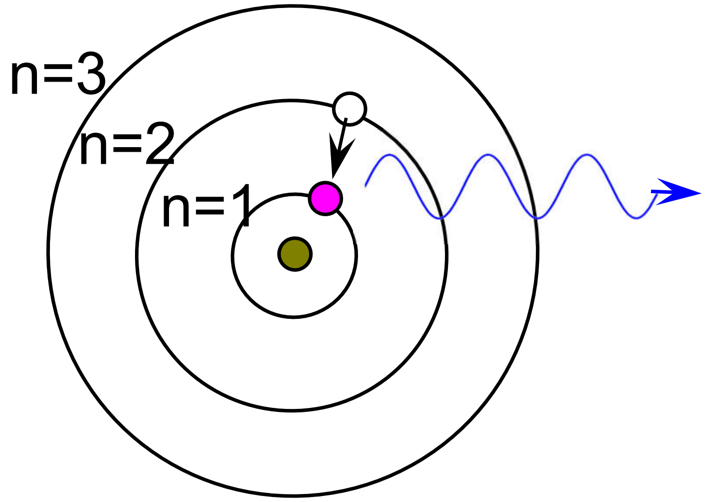
This plasma is mostly hydrogen and pretty cold.

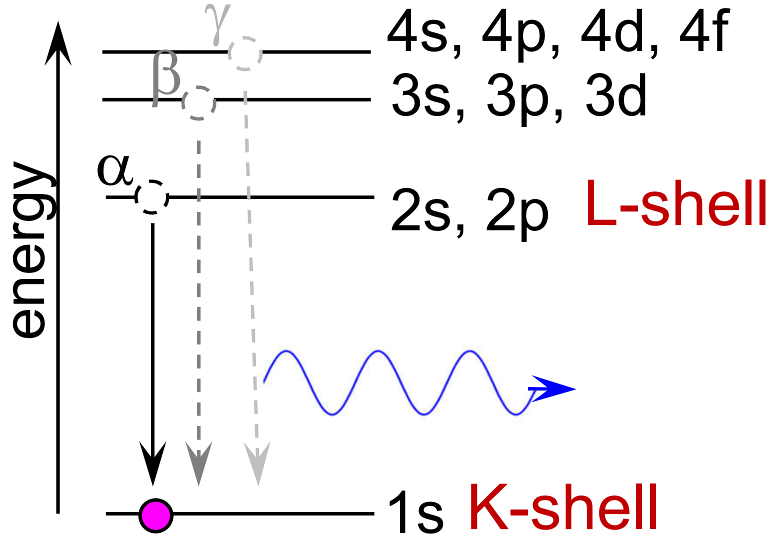


Each ion of each element has a spectroscopic “fingerprint”

Bohr model:

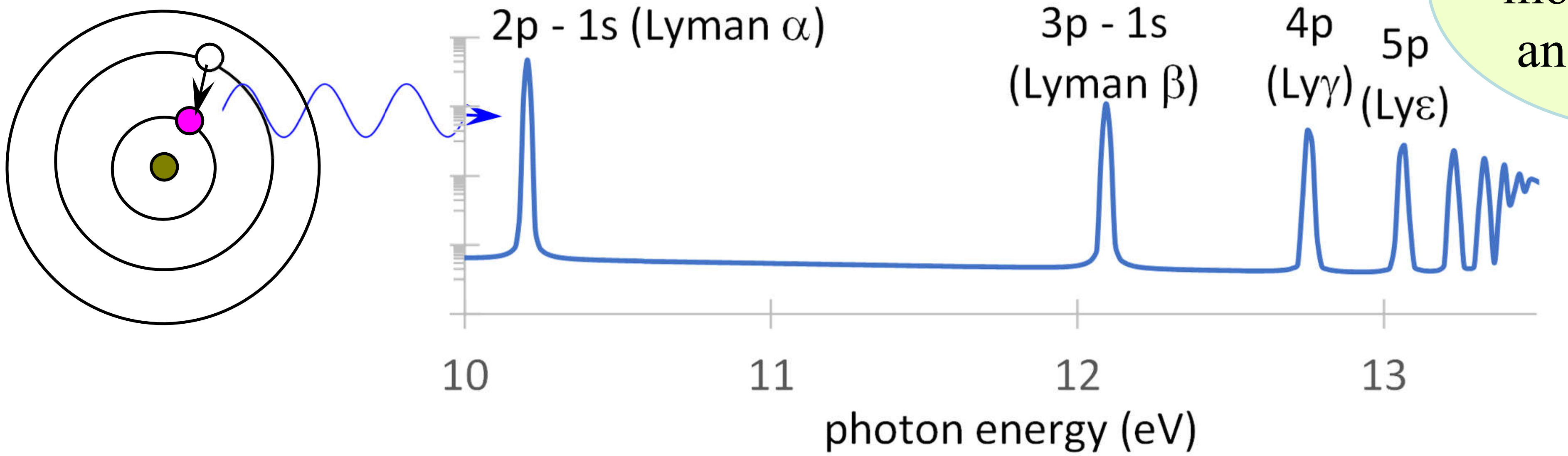
$\varepsilon_n \sim 13.6\ \mathrm{eV}\ (Z_{eff}/n)^2$



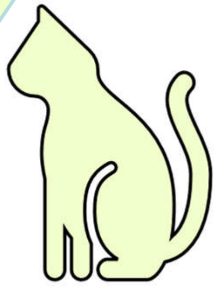


neutral hydrogen ($Z = 1$, n = 1)

K-shell hν = Δε ~ 10 eV

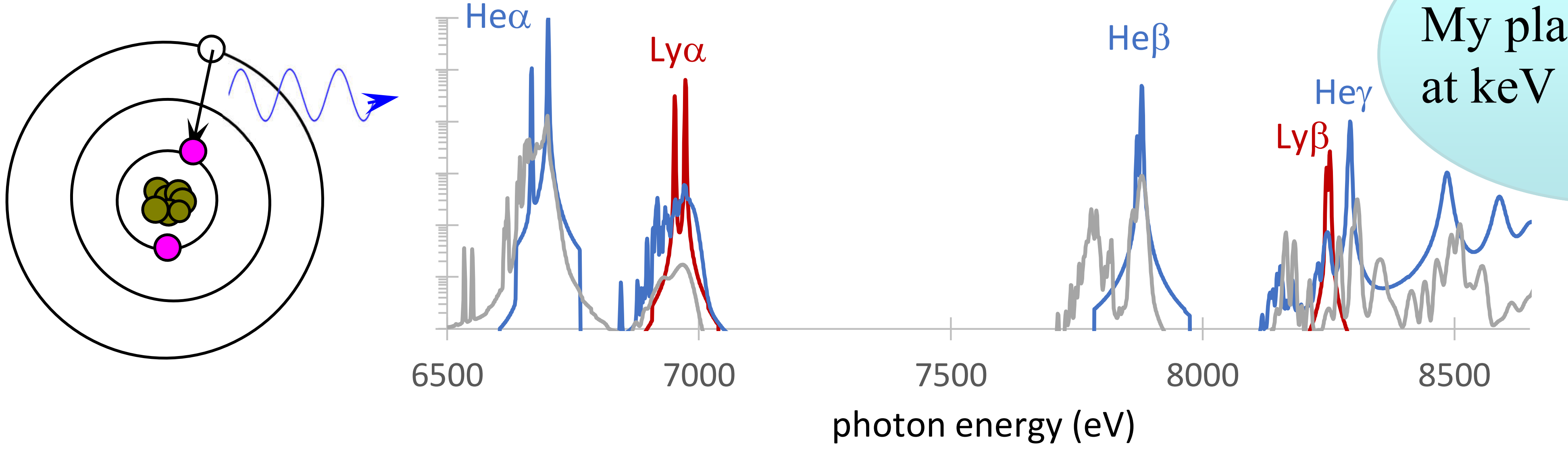


This plasma is mostly hydrogen and pretty cold.

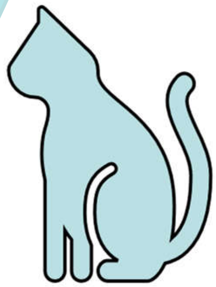


He-like iron (Z_{eff} ~ 25, n = 1)

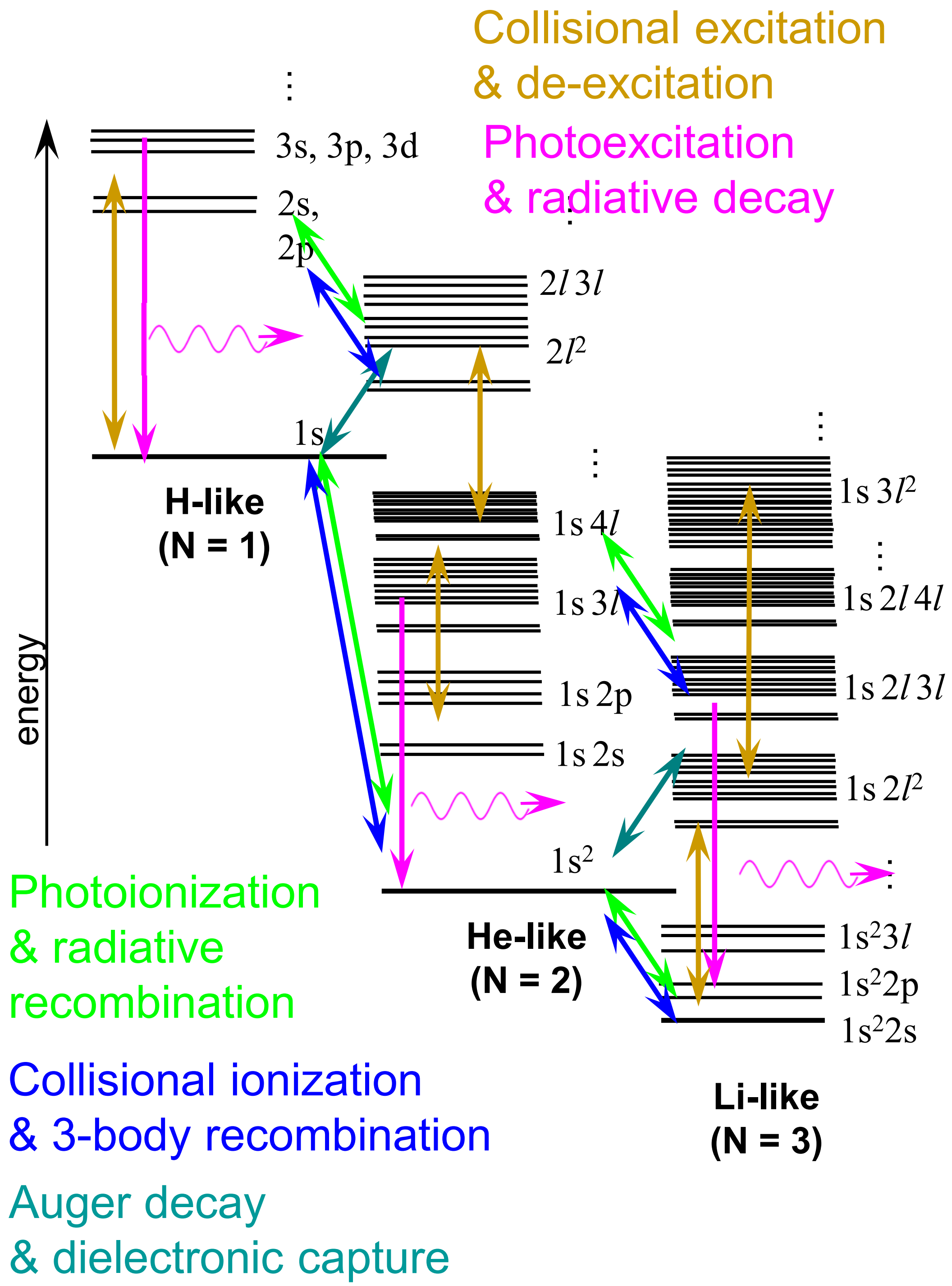
K-shell hν = Δε ~ 7000 eV



My plasma has iron at keV temperatures!



And unfortunately, not many high-temperature plasmas are in Local Thermodynamic Equilibrium (LTE)



Collisional excitation & de-excitation

Photoexcitation & radiative decay

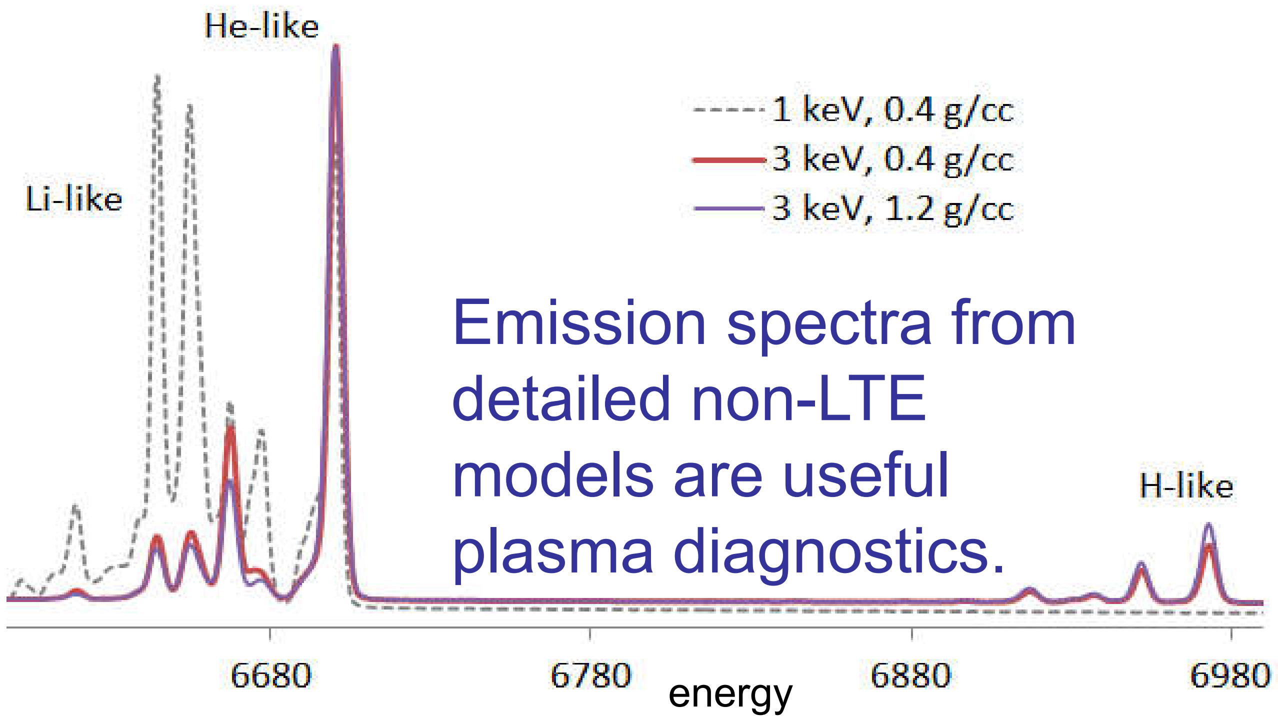
Photoionization & radiative recombination

Collisional ionization & 3-body recombination

Auger decay & dielectronic capture

LTE enables simple statistics for populations, but only for simple environments ($T_e = T_{ion} = T_{rad}$, $dX/dt = 0\ldots$)

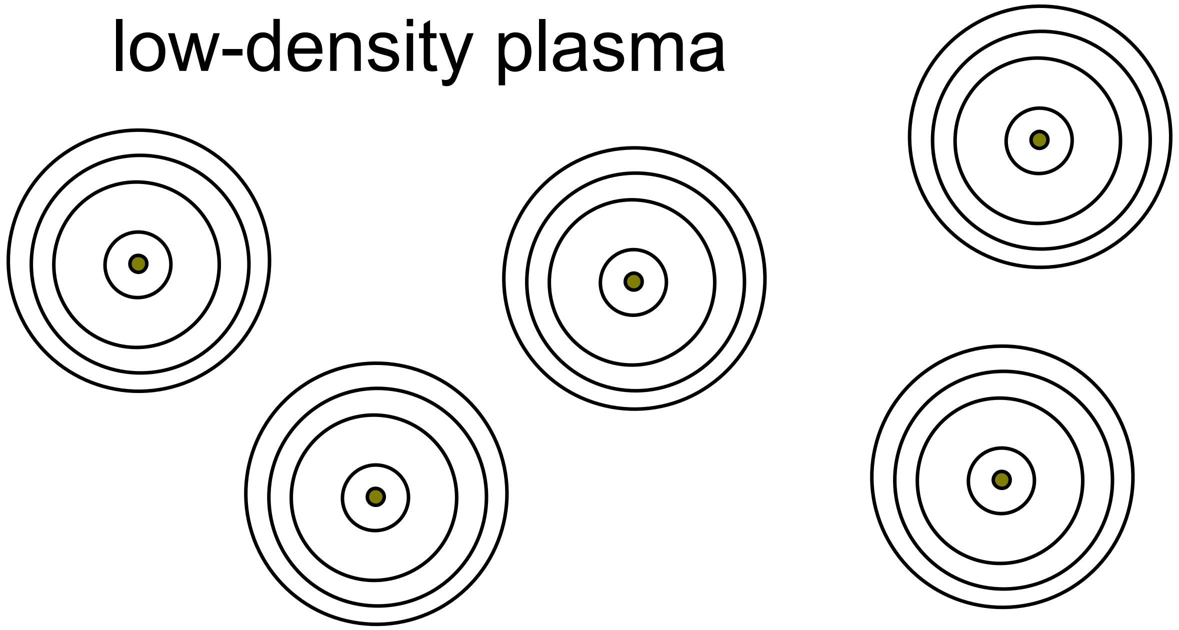
Each non-LTE plasma is non-LTE in its own way and requires solving a set of coupled rate equations that grows larger with increasingly complex atomic structure



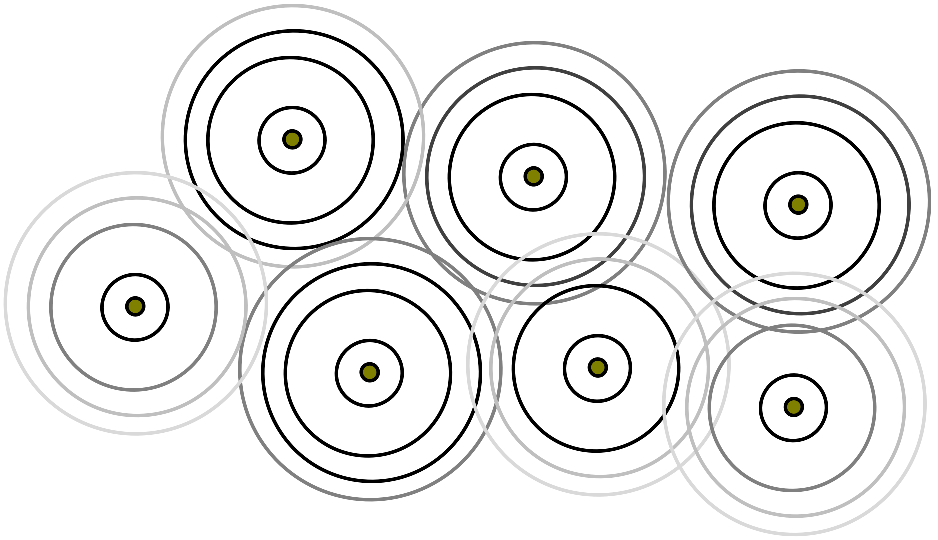
Emission spectra from detailed non-LTE models are useful plasma diagnostics.

And unfortunately, not all ions are isolated: High-density environments modify electronic structure

low-density plasma

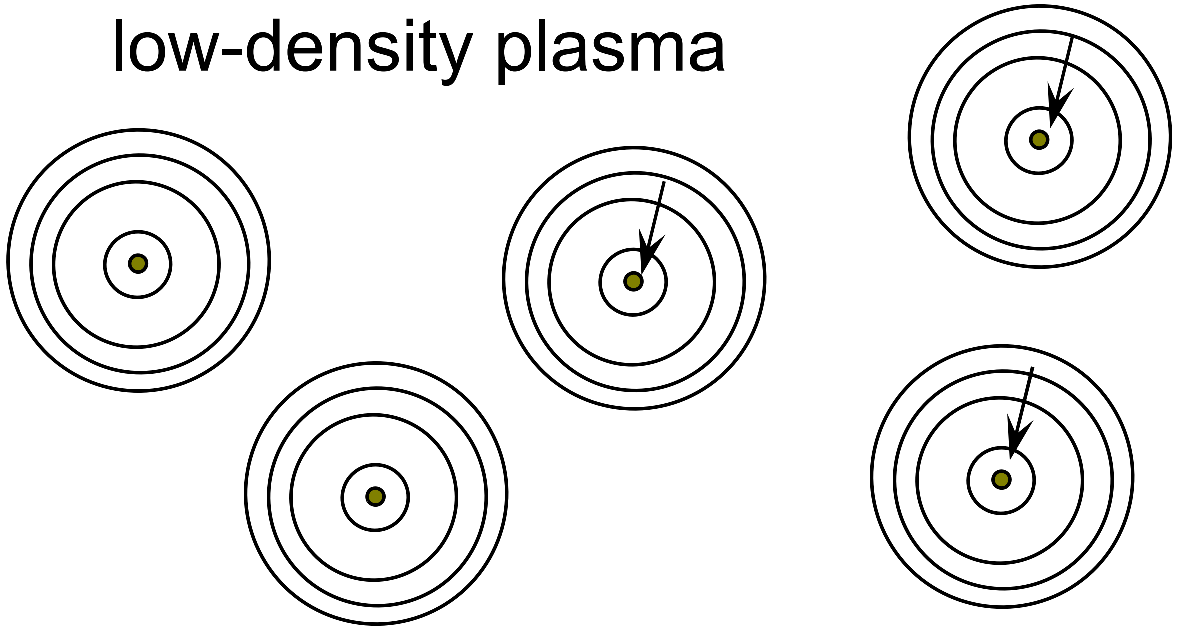


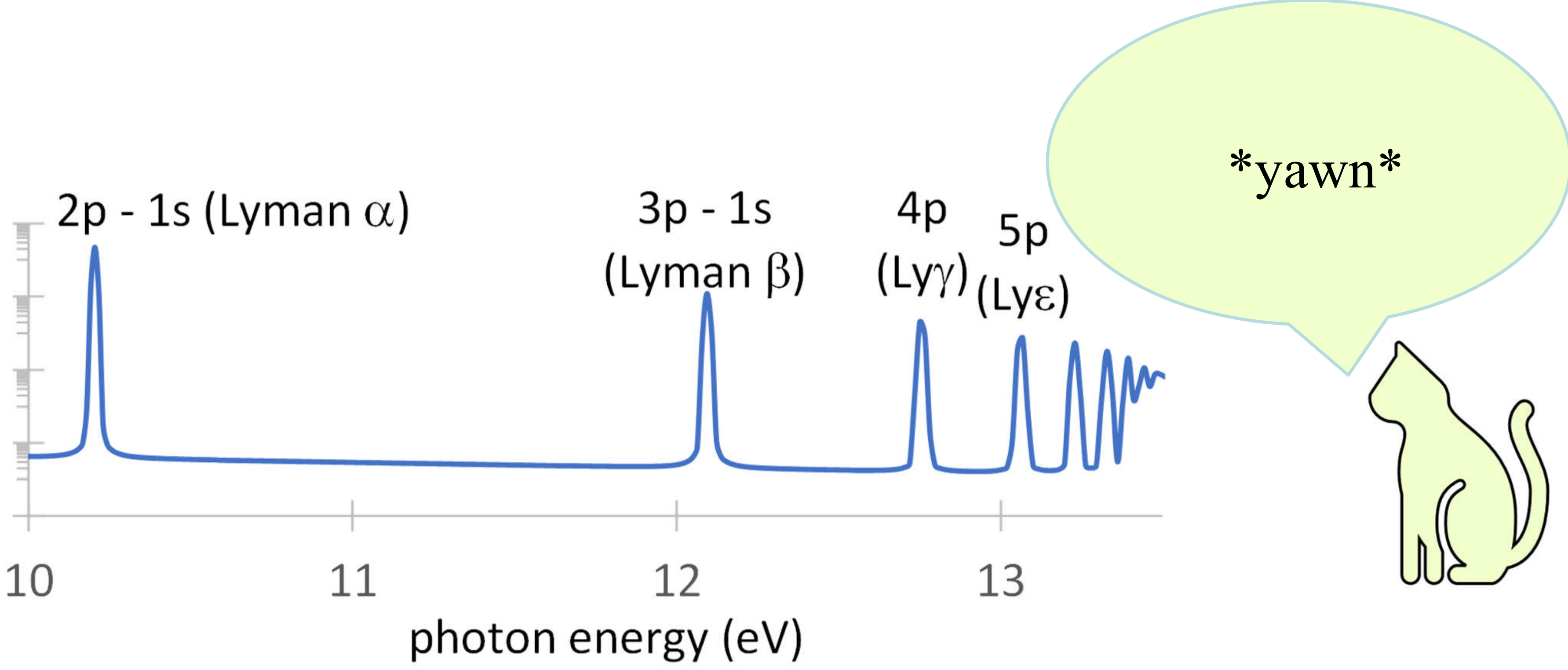
high-density plasma



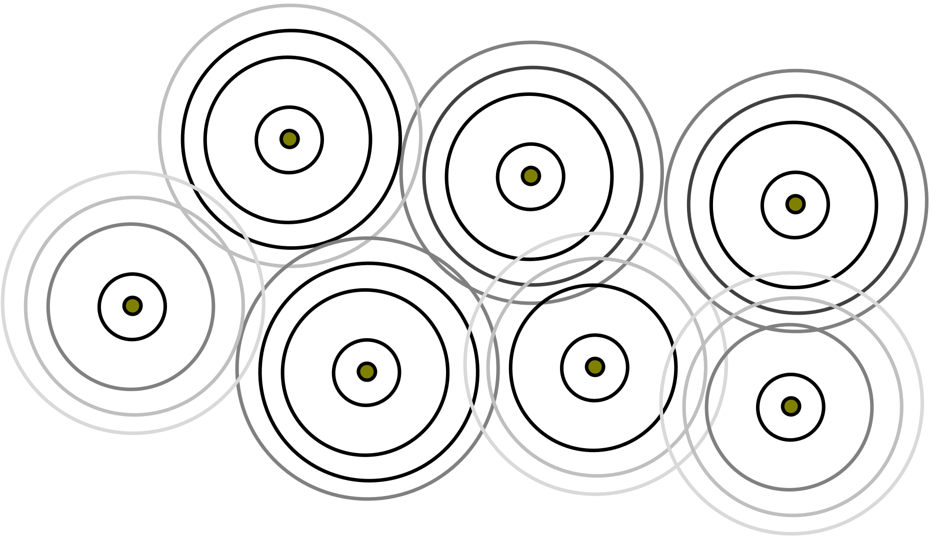
High-density environments modify electronic structure

low-density plasma



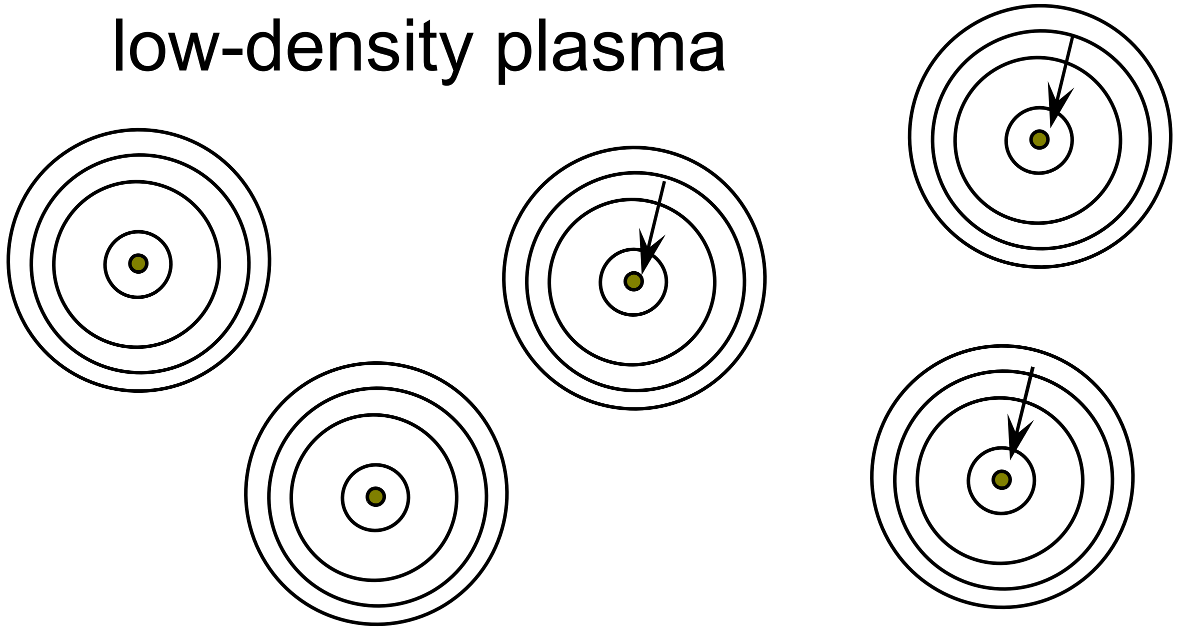


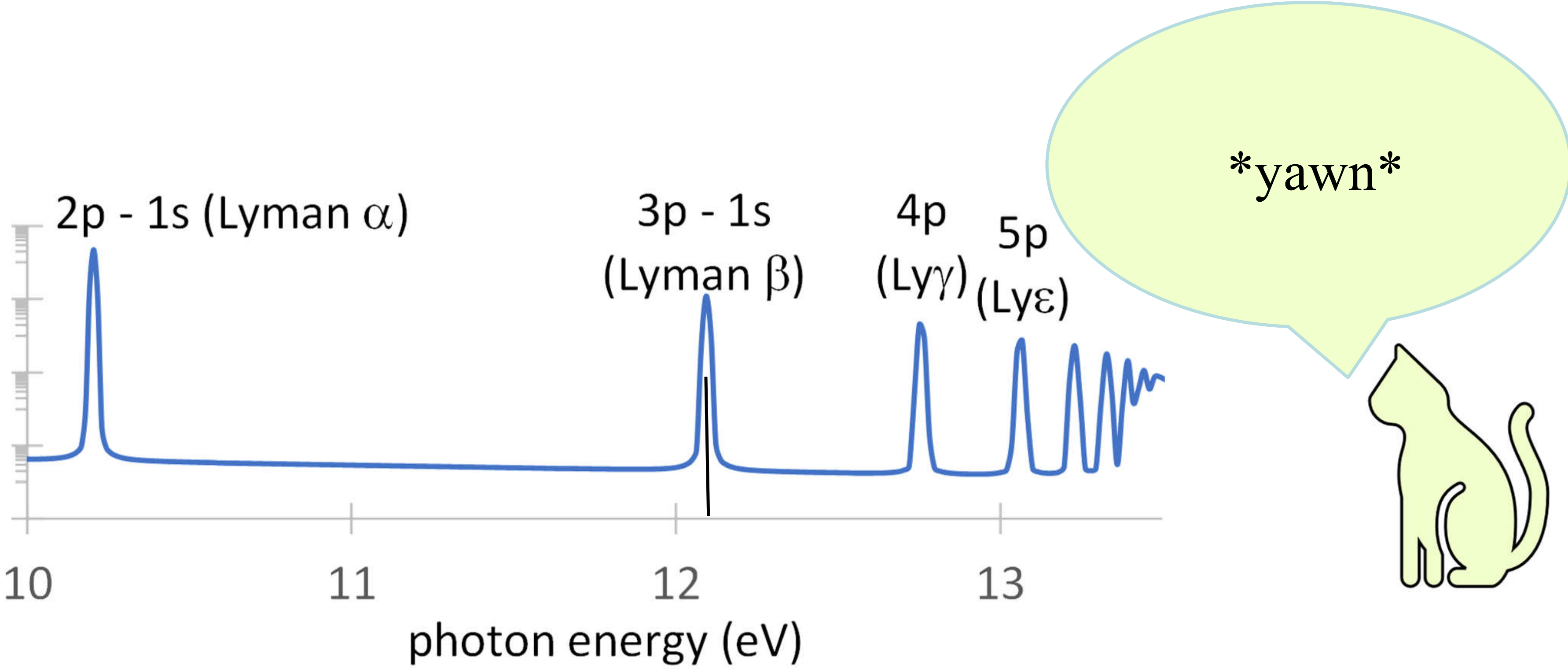
high-density plasma



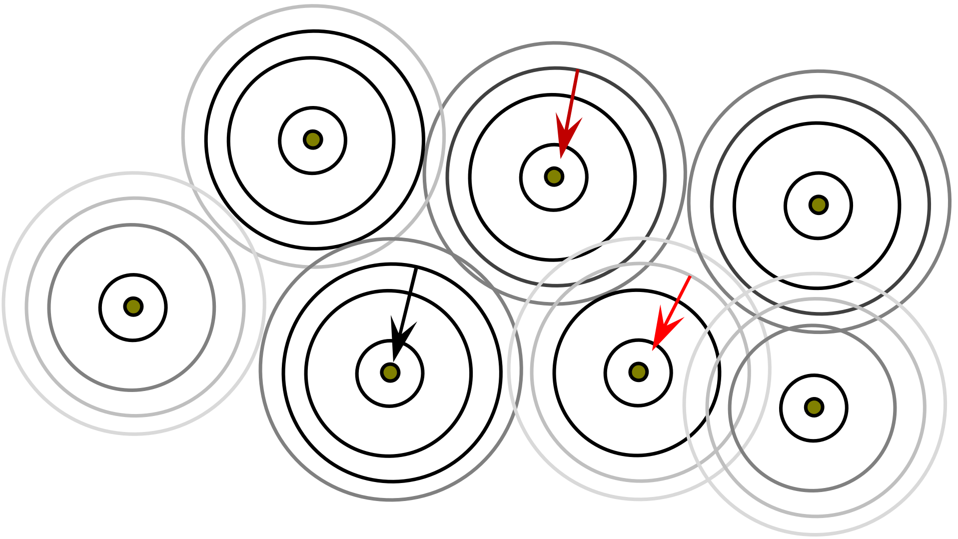
High-density environments modify electronic structure and spectroscopic signatures

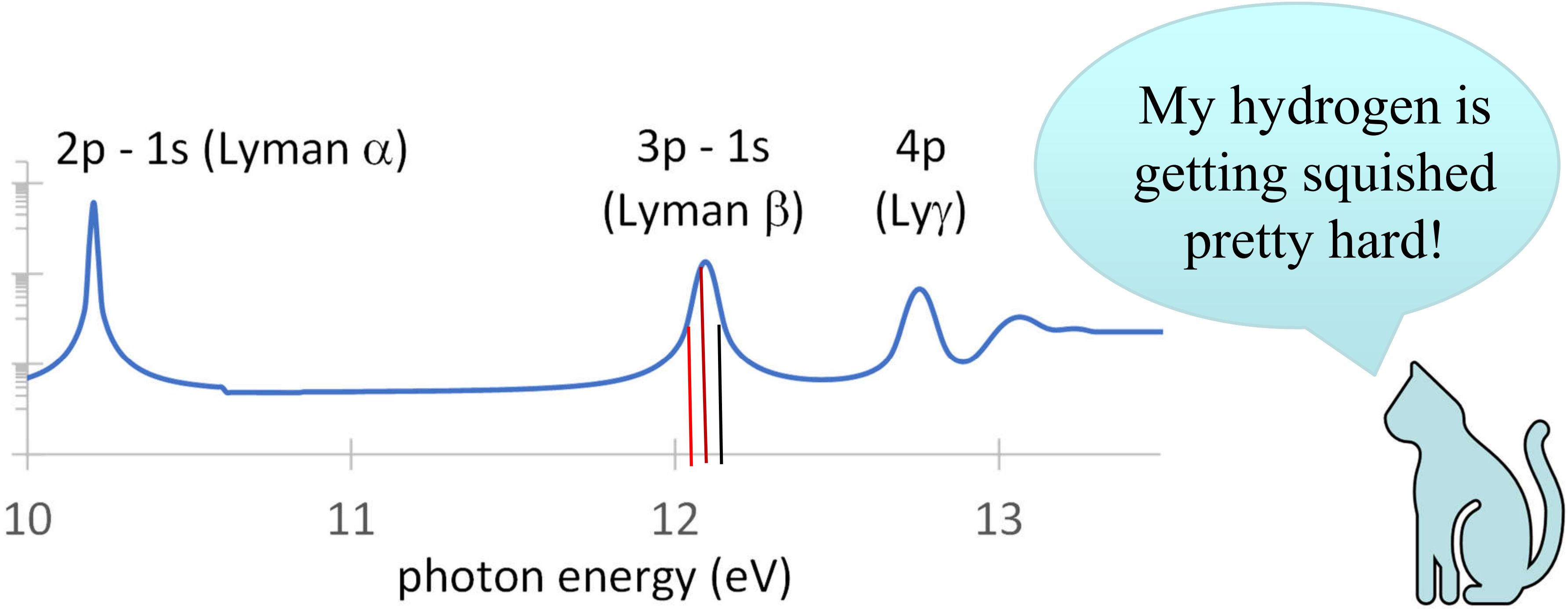
low-density plasma





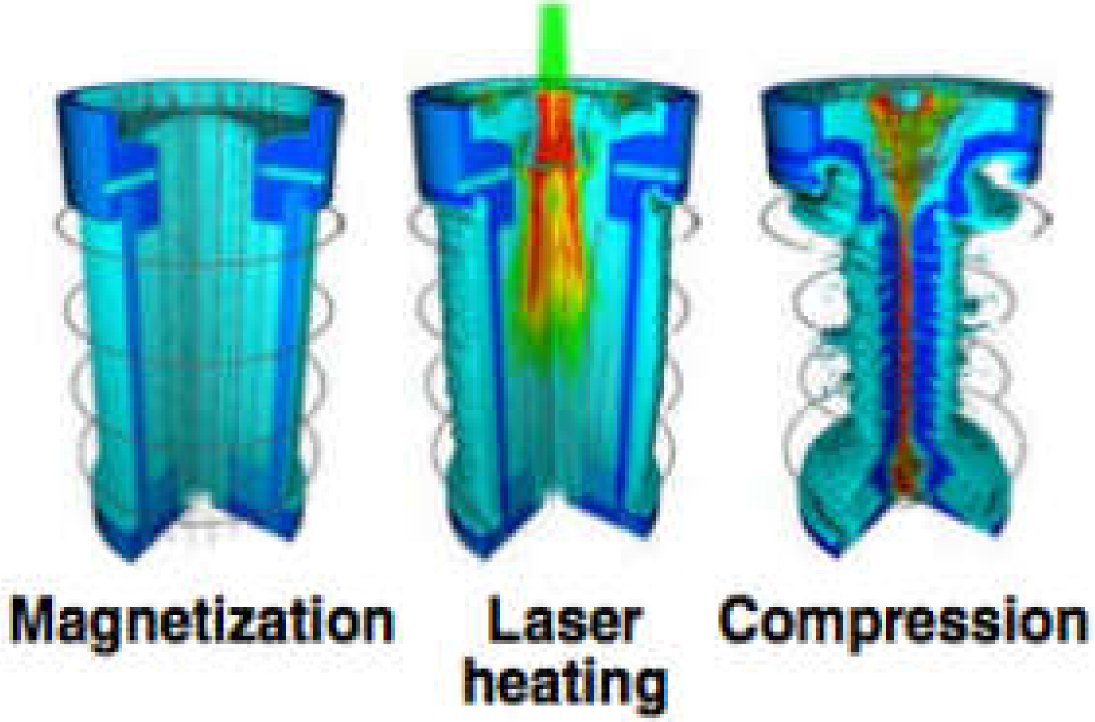
high-density plasma

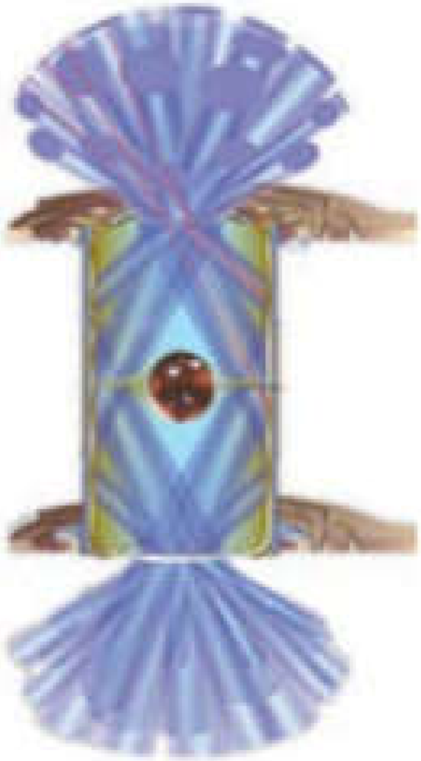


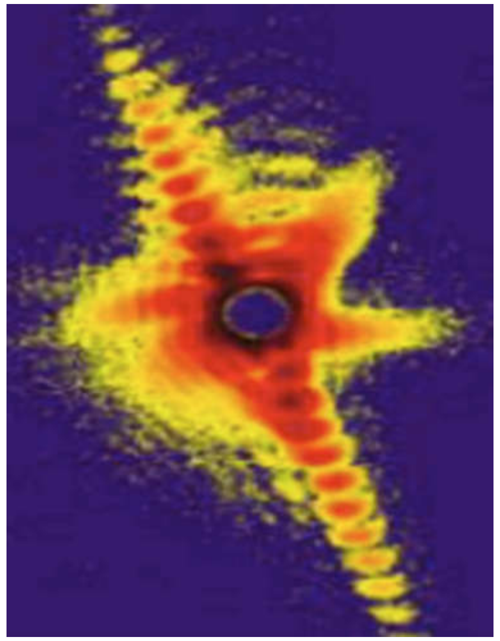


How do we produce extreme conditions in the laboratory?

We compress energy in space and time using pulsed power, lasers, or undulators





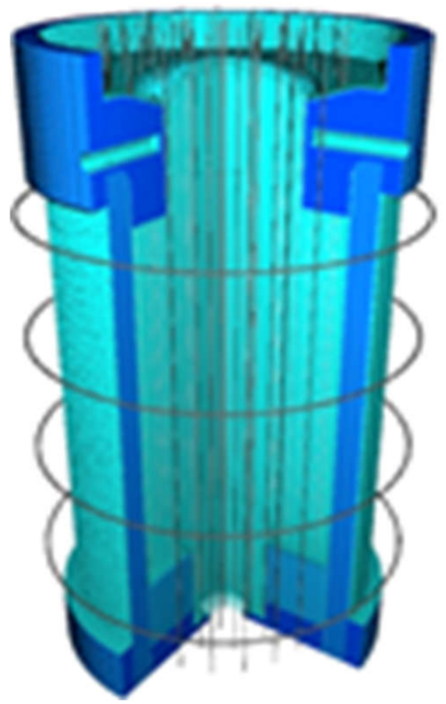


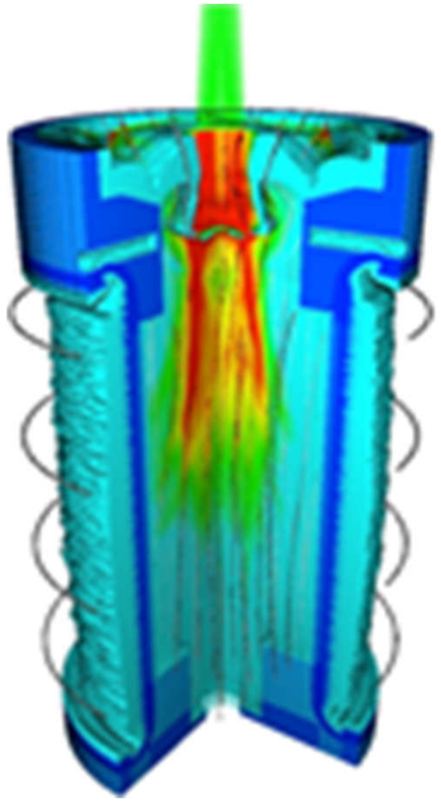
SNL's Z machine:
10 MJ → 10^{-9}s, 100-1000 μm
0.3 - 3 keV, 0.01 – 1 g/cc
~2 kJ fusion
>100 TW x-rays
fundamental HED science

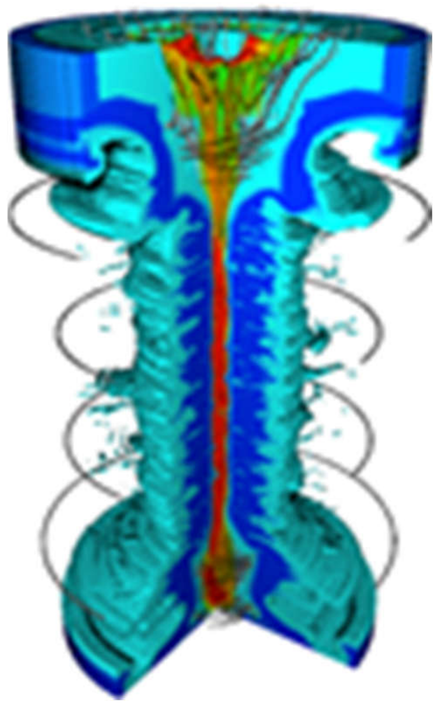
LLNL's NIF:
2 MJ → 10^{-10}s, 10-100 μm
0.3 - 3 keV, 0.01 – 100 g/cc
~20 kJ fusion
bright x-rays
fundamental HED science

LCLS/ European XFEL:
2 mJ → 10^{-13}s, 1μm
10 eV, 1 – 10 g/cc
fundamental science

Sample application: Magnetized Liner Inertial Fusion (MagLIF)







Premagnetization:
External Bz field inhibits thermal conduction losses

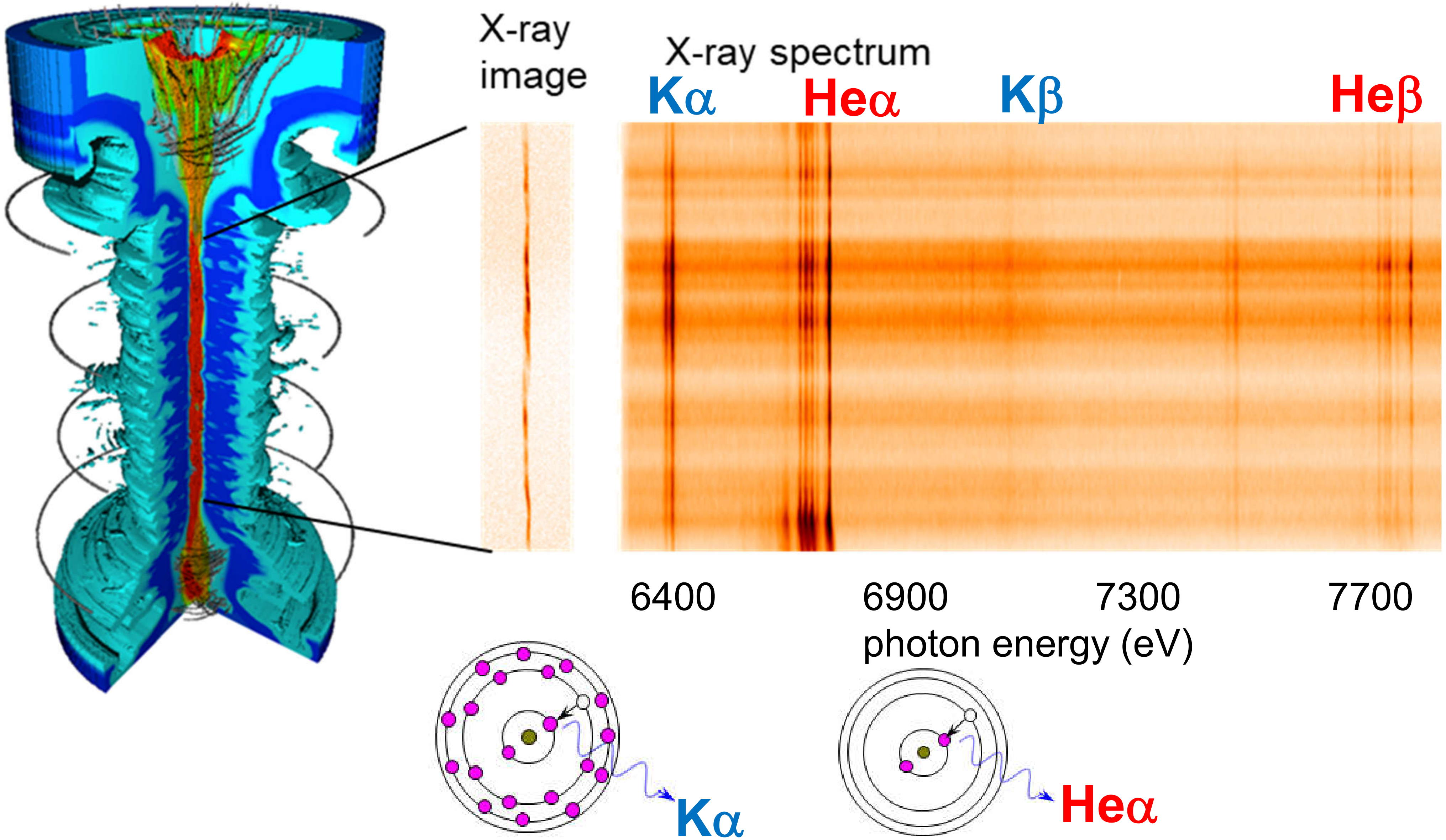
Laser preheat:
Allows slower, more stable implosions (high adiabat)

jxB implosion:
Heats fuel to fusion temps; compressed Bz traps charged fusion products

Simulations courtesy C. Jennings

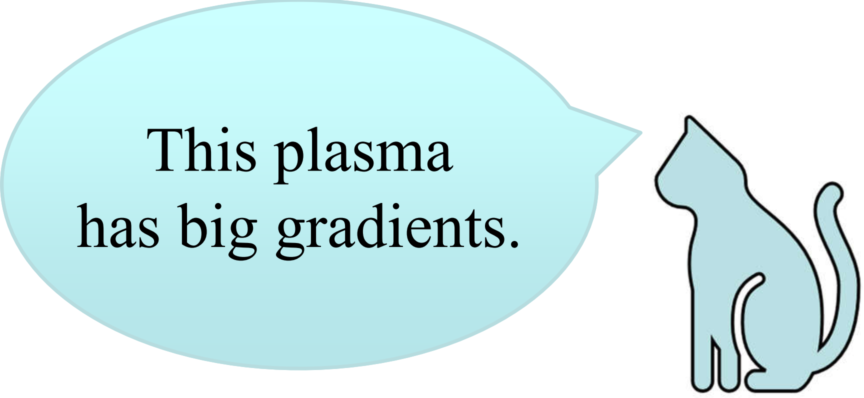
What does the spectrum from a MagLIF experiment tell us?

MagLIF is a Be liner with ~100 ppm Fe impurities surrounding a pure-D2 fuel core



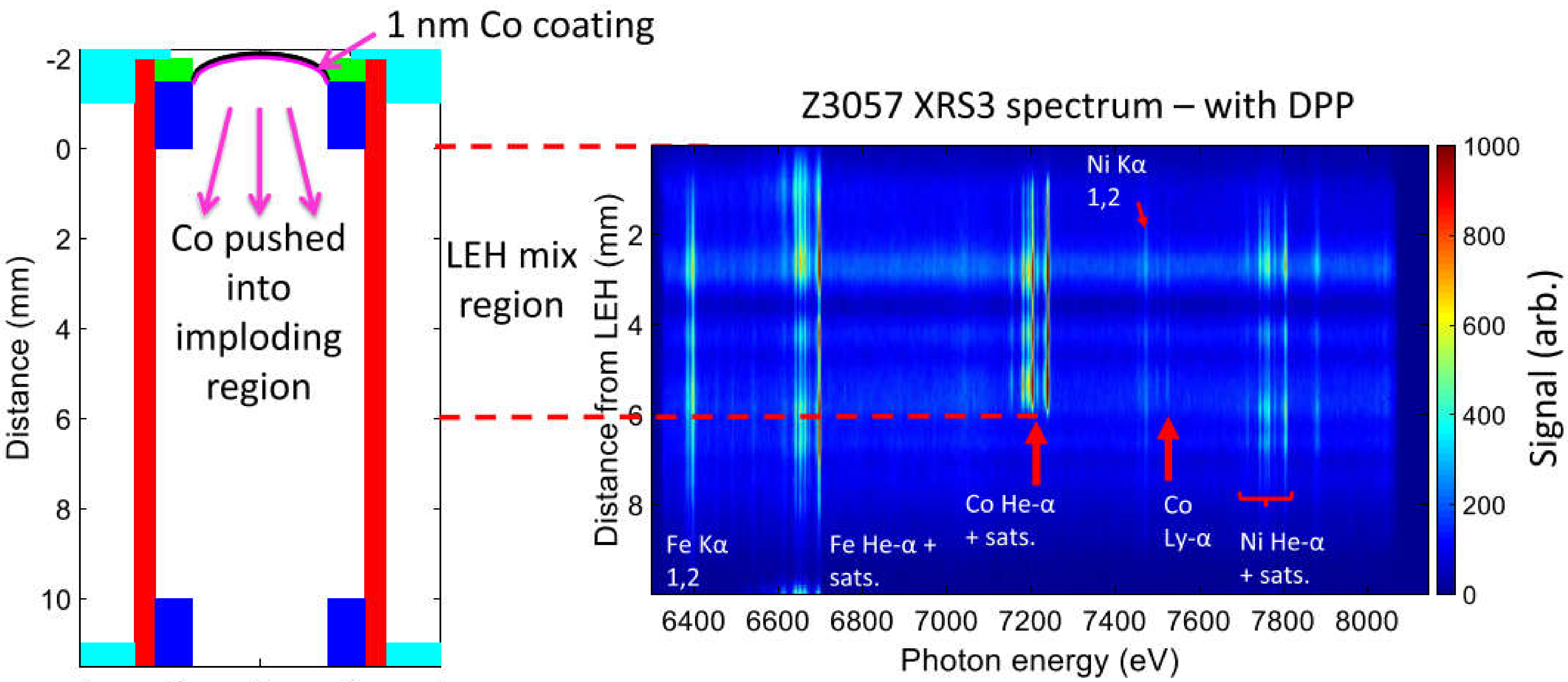
He-like iron K-shell lines: some of the liner mixes with the hot fuel in a layer with n_e ~ 2×10^{23} e/cc and T_e ~ 2000 eV

Neutral iron K-shell lines: most of the liner is cold (~10 eV) and very dense (10x solid): the iron is photoionized by radiation from the hot core

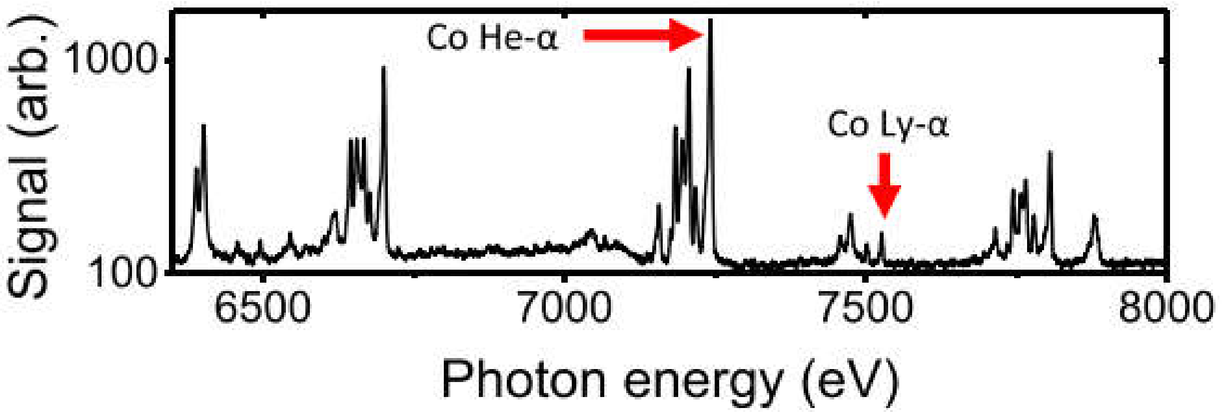


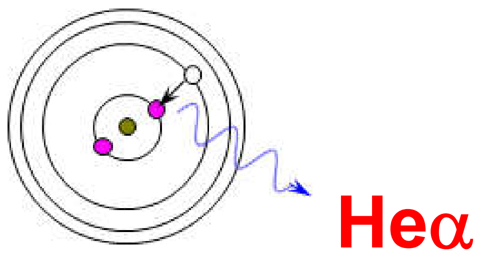
Spectrum Courtesy E. Harding

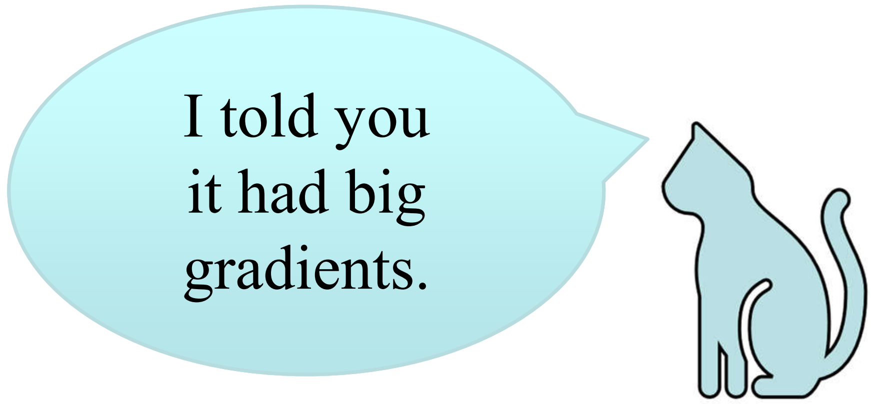
Is the whole hot core at the same conditions as the hot iron?



No! When we put a cobalt tracer on the window and use a smoothed, large-area beam to preheat, the window material pushed into the fuel indicates hotter (4 keV) and less dense (10^{23} cm^{-3}) plasma







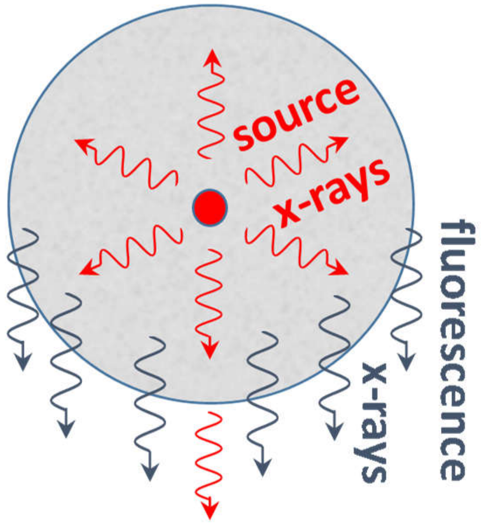
A. Harvey-Thompson, Phys Plas 25, 112705 (2018)

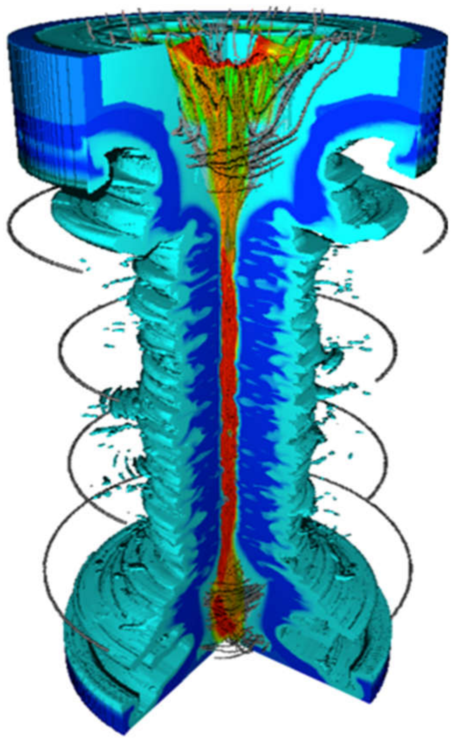
Fluorescence emission from iron impurities confirm significant gradients and reveal density effects

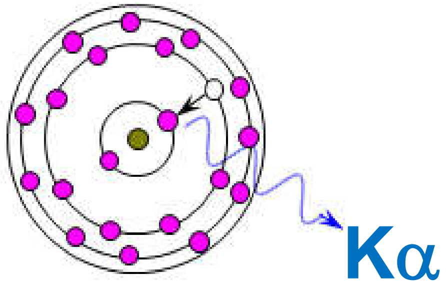
A pronounced shift in the cold Kβ (3p – 1s) line of iron impurities indicates liner is at a high density, compressed to ~8x solid

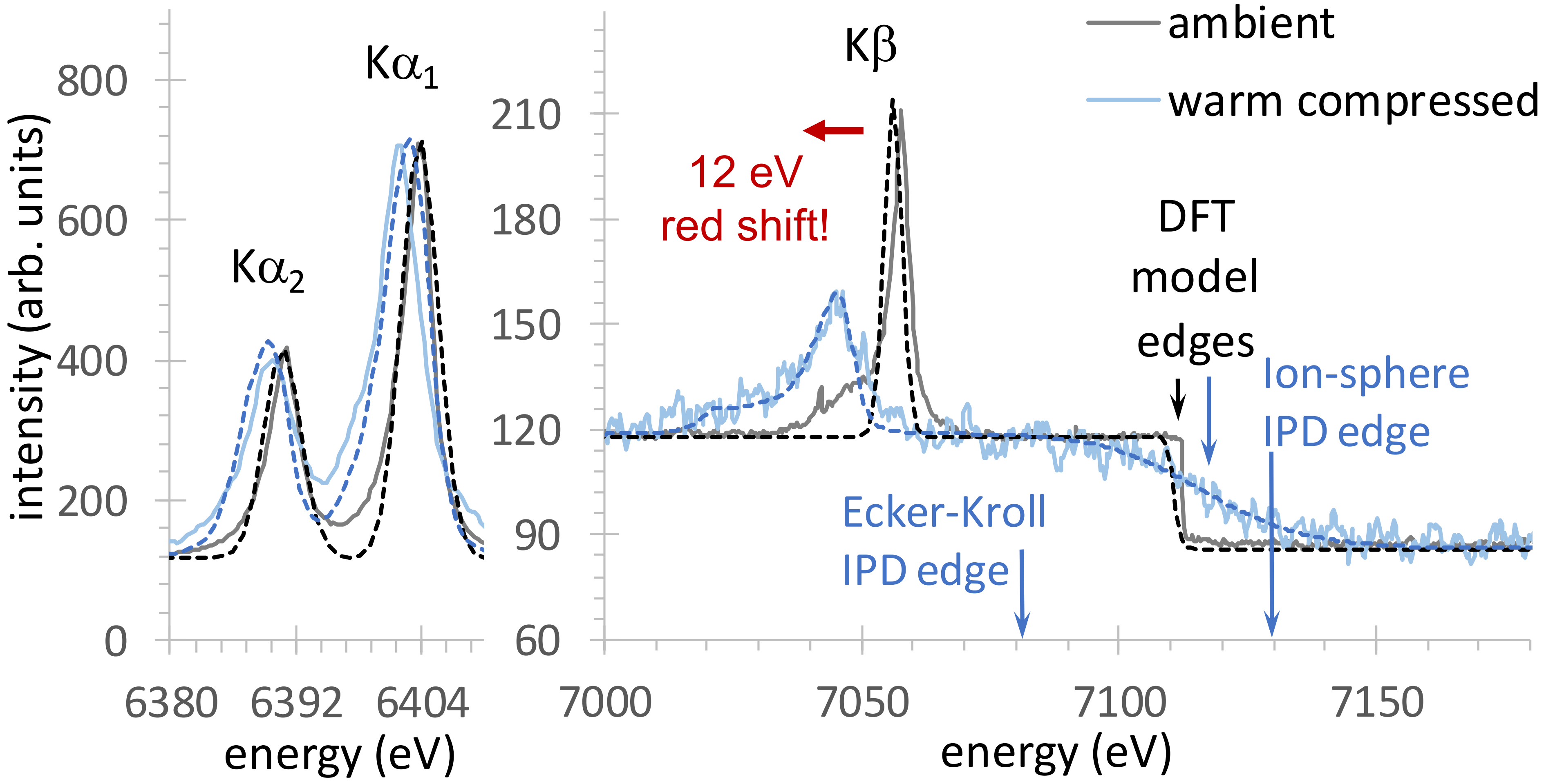
The slope of the iron K-edge indicates Te ~ 10 eV, depth confirms compression

High-precision spectra help us distinguish between models of density effects





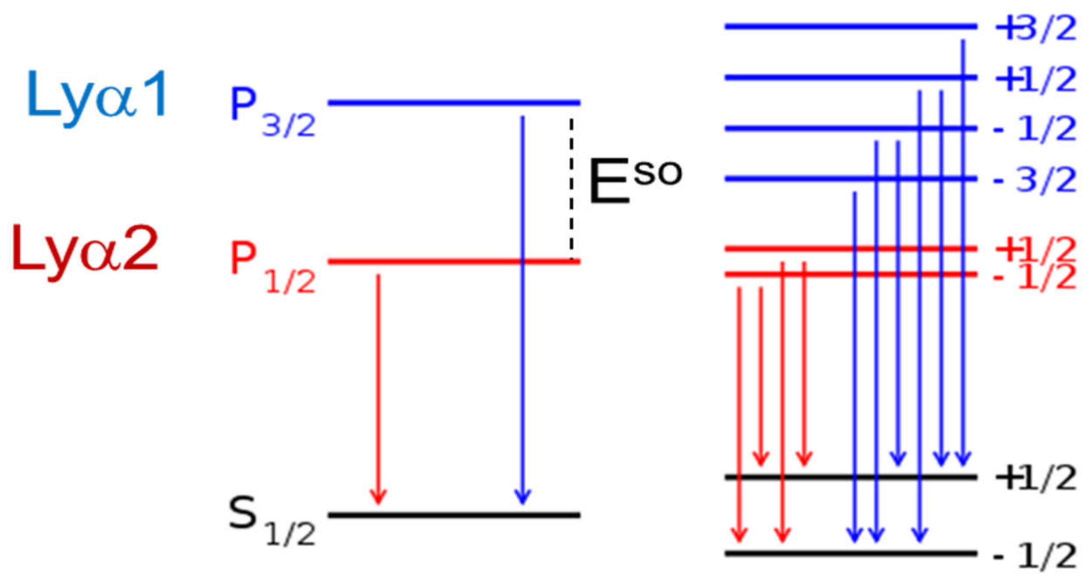




Dashed lines are models, solid lines are measurements*

*Hansen et al, Phys Plasmas 2017

Differential splitting can help us constrain flux-compressed magnetic fields at stagnation

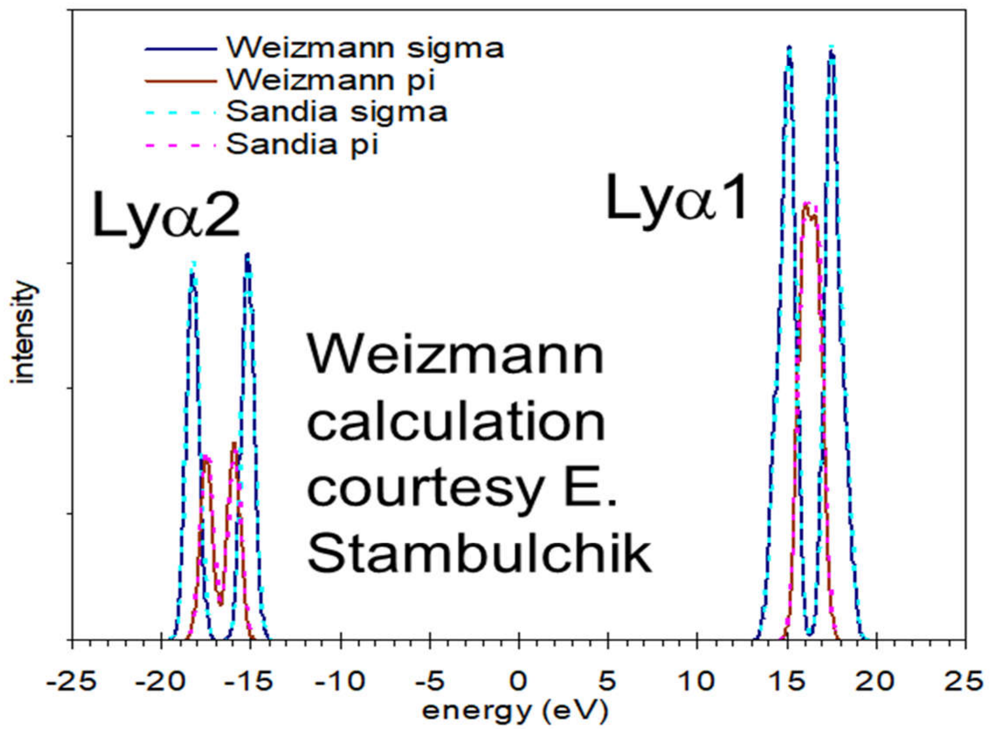


Zeeman splits Lyα2 more than Lyα1
Maron et al Phys Plas 18, 093301 (2011)

Uniform, lossless compression @ CR 40 → 15 kT
Nernst would increase expected field near edge
Flux losses would decrease expected field

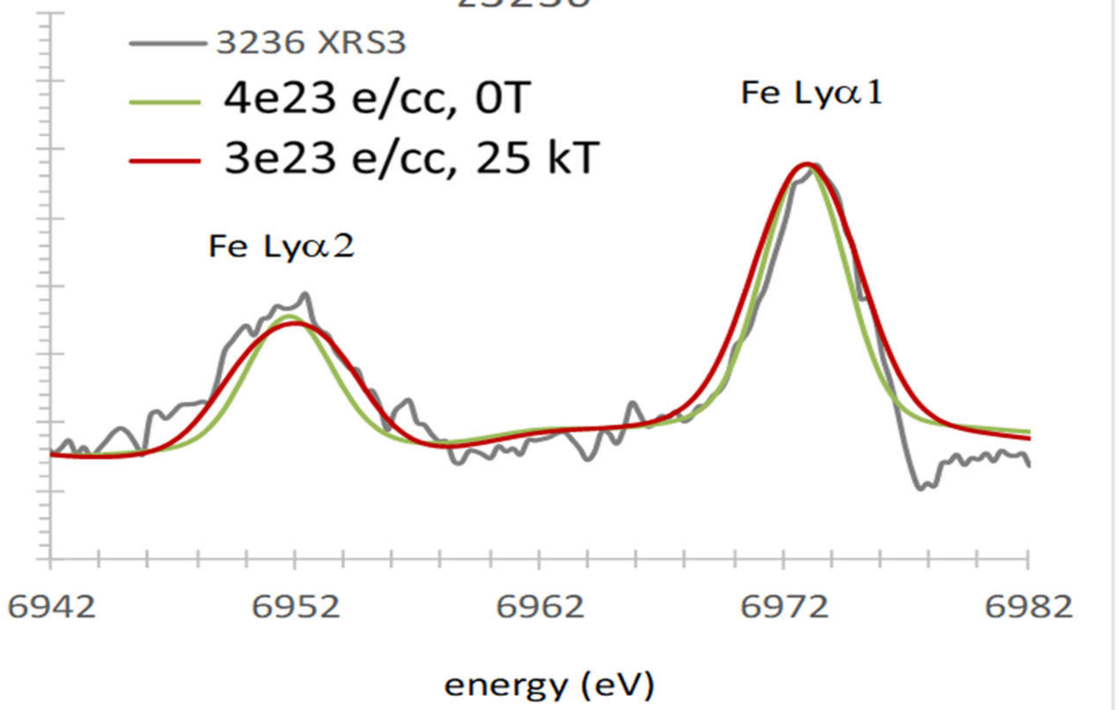
With Co in window & high T in central stagnation for Co Lyα, we might be able to infer Bz(r) and inform Nernst

Cu Lyα; B = 2×10^4 T ($E^B < 0.1\ E^{SO}$)

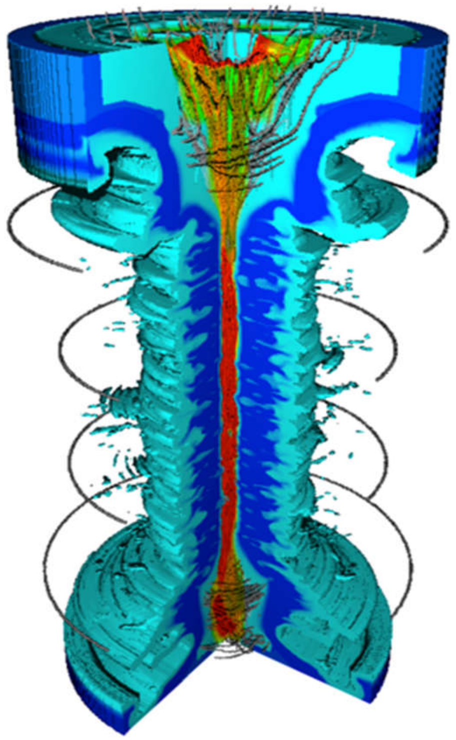


Weizmann calculation courtesy E. Stambulchik

z3236



Combining these spectroscopic diagnostics, we can build up a detailed picture of MagLIF at stagnation



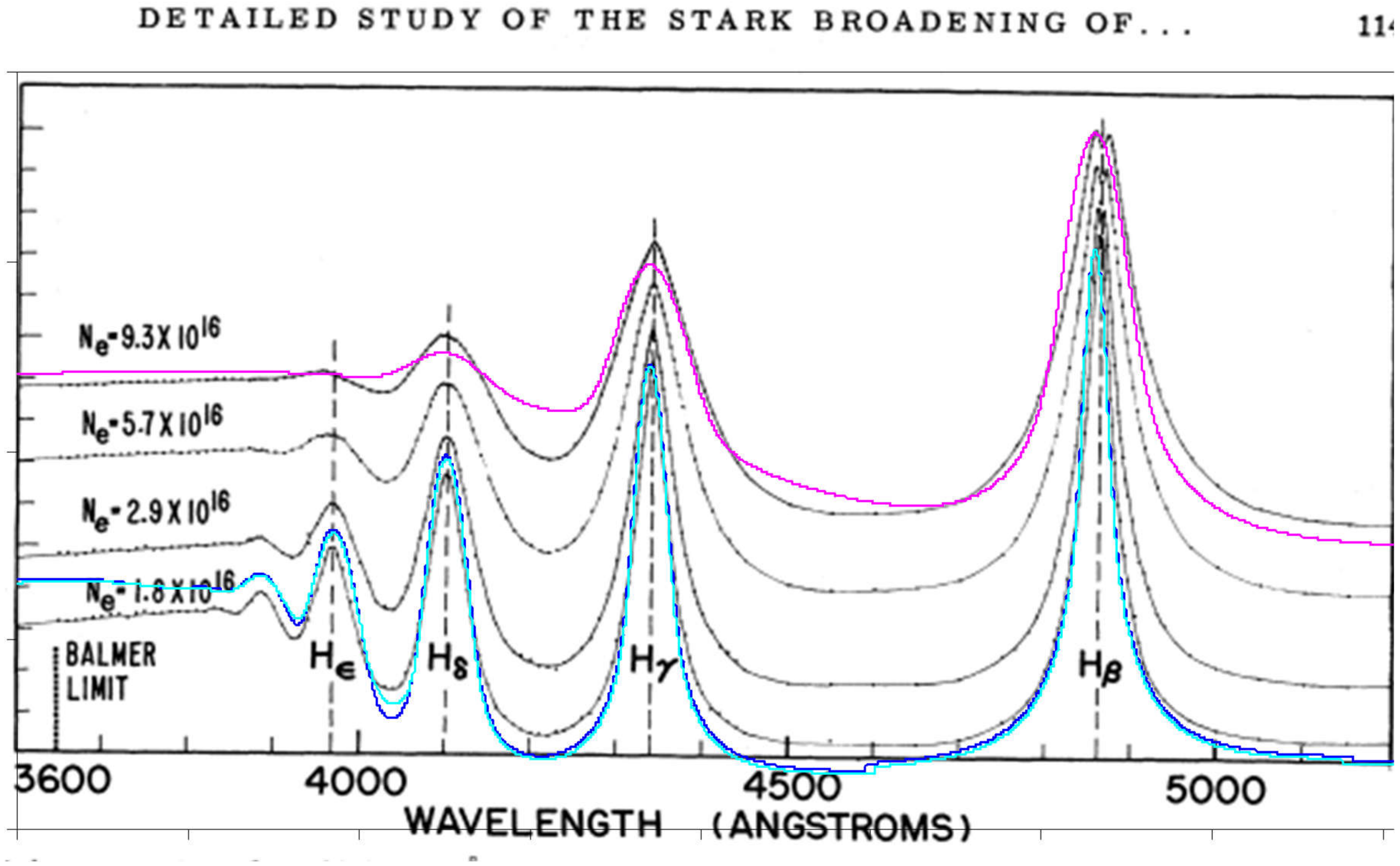
1) hot core with: ne ~10^{23} e/cc, Te = 3-4 keV, & Bz ~ 20 kT
2) warm mixed layer with ne ~ $2x10^{23}$ e/cc, Te = 1- 2 keV
3) cool, compressed liner with ne ~ $2x10^{24}$ e/cc, Te = 10-20 eV

This detailed picture helps us rigorously validate rad-MHD simulations and understand the impact of target design changes

How do we know if our atomic-scale models are reliable?

We can test them in careful, “benchmark” experiments with plasma samples that are:

1. designed to be relatively uniform
2. independently characterized
3. carefully diagnosed



Wiese, Kelleher, and Paquette, *Phys. Rev. A* **6**, 1132 (1972)

Hydrogen at T ~ 2 eV:

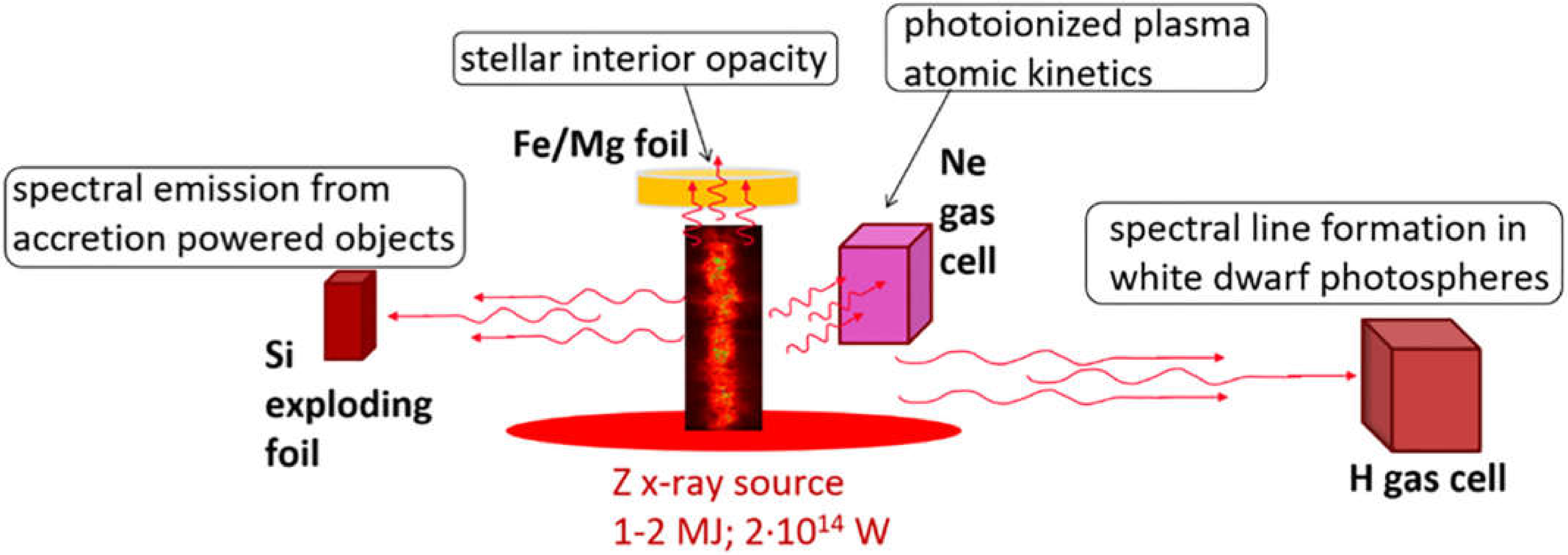
*one of perhaps **5** high-quality benchmark data sets for spectra!*

High-quality benchmark experiments are difficult but *enduring* (and highly cited!)

The closer you get to literal “benchmark” experiments (a lump of iron on your bench), the better!

Opportunity: warm dense matter (WDM) is experimentally accessible and computationally complex

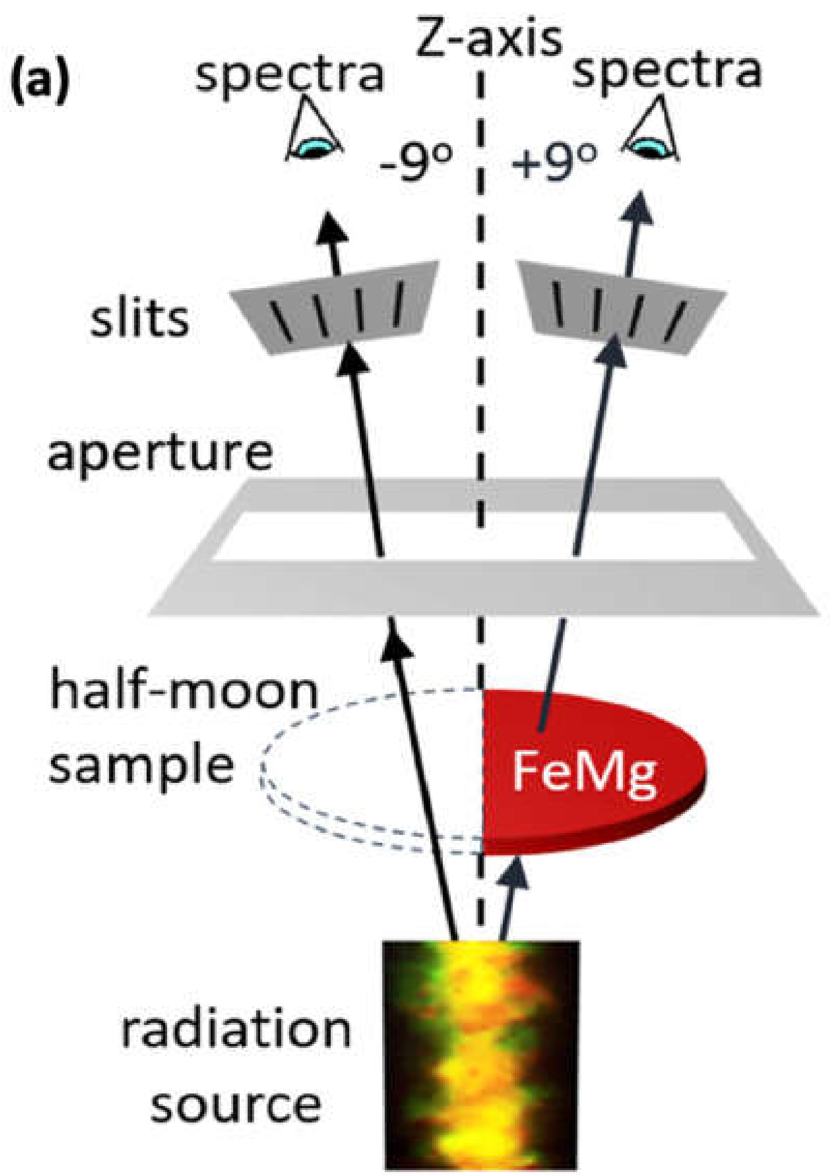
The Z Astrophysical Plasma Properties (ZAPP) collaboration aims to benchmark extreme, astrophysically relevant plasmas



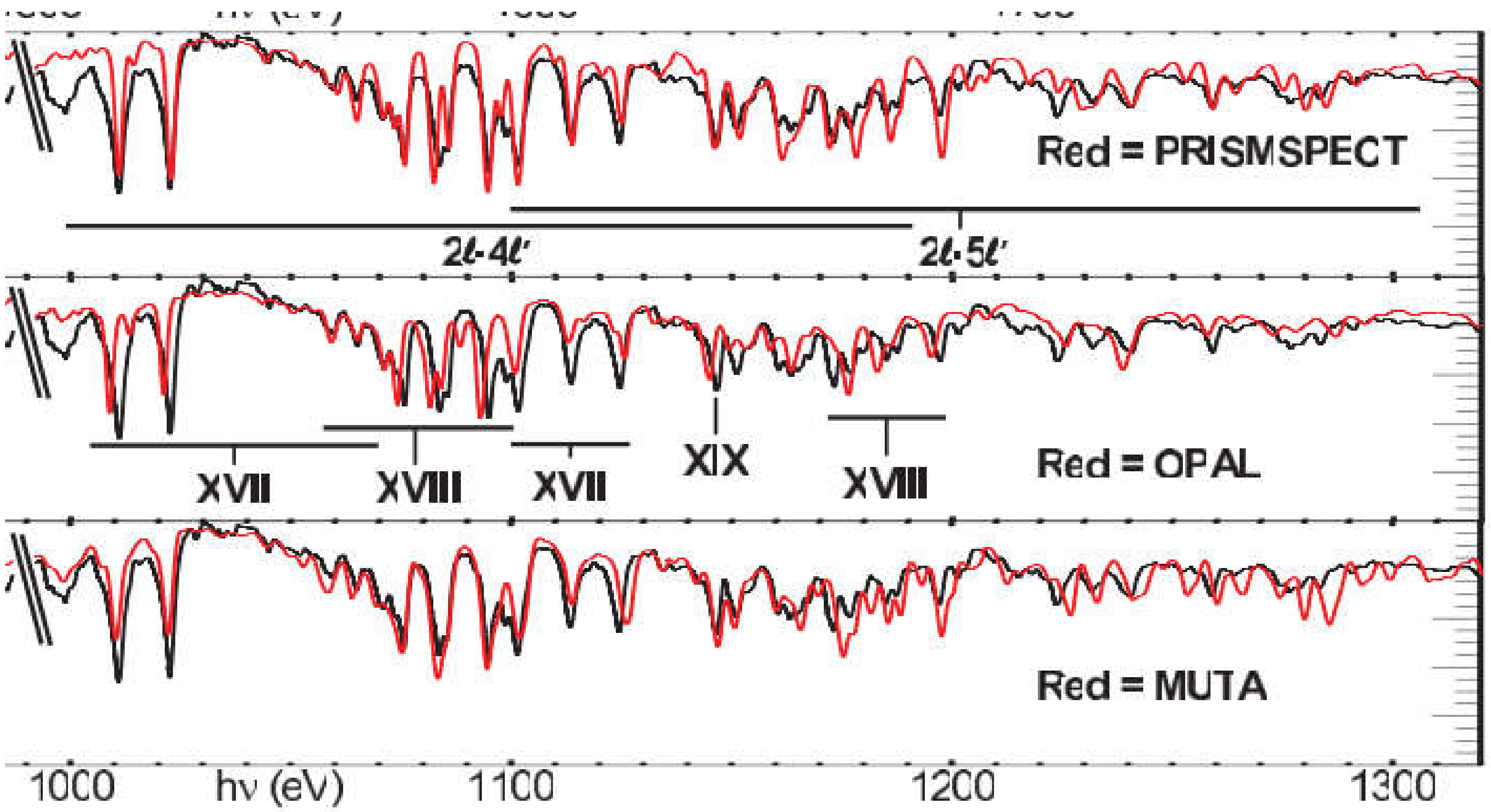
A consortium of Laboratory and University scientists use the TW x-ray powers from the Z machine to heat, photoionize, and backlight benchmark plasmas

Rochau, G. A. et al. Phys. Plasmas 21, 056308 (2014)

Benchmark measurements of stellar interior opacities inform models of our sun (helioseismology, elemental abundances)

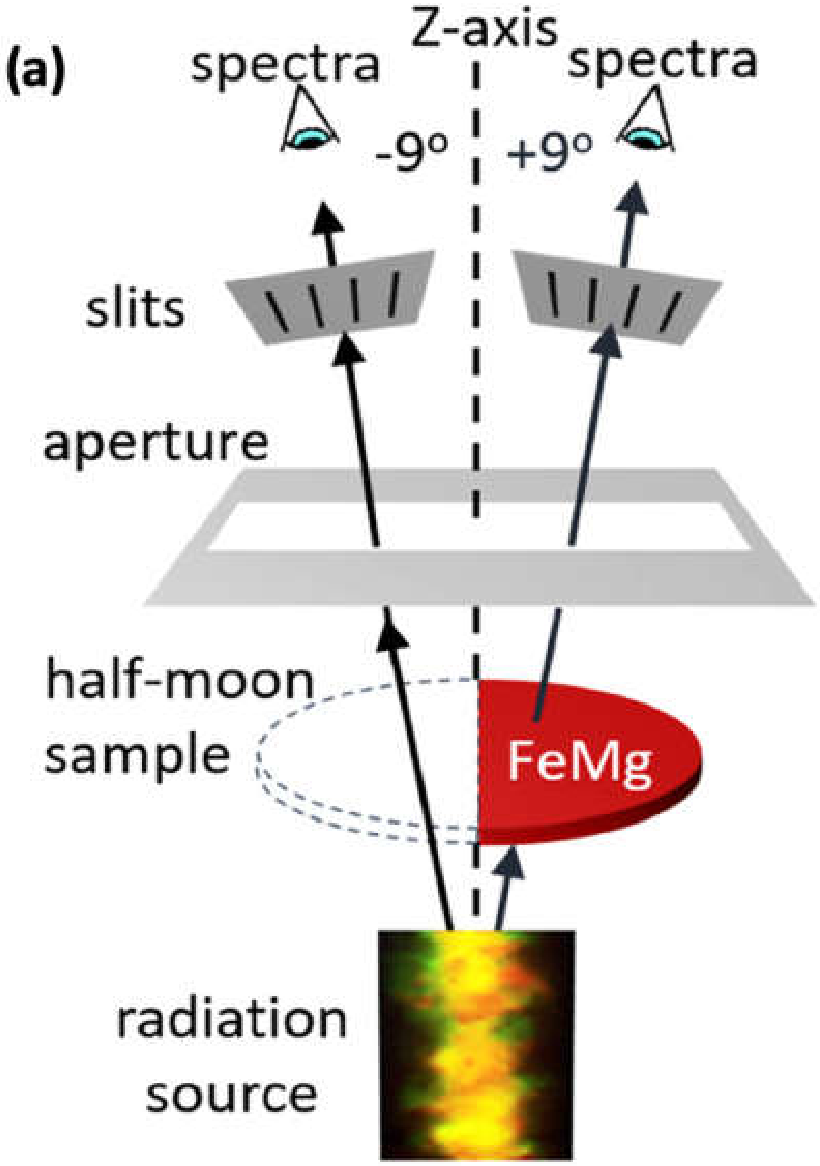


In 2007, Bailey at al found good agreement between models and experiments for iron at temperatures and densities slightly lower than that at the solar radiation/convection zone boundary:

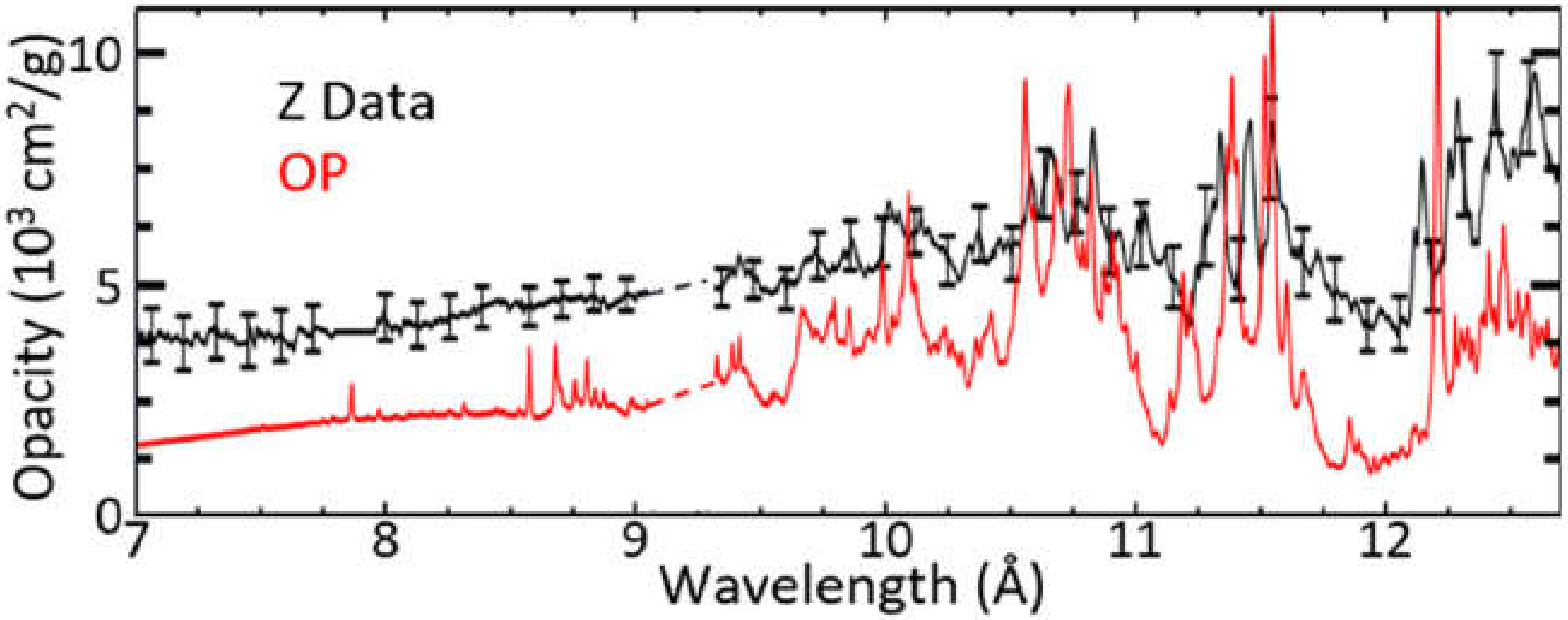


Bailey et al, Phys Rev Lett 99, 065002 (2007)

More recent measurements show discrepancies with models at more extreme conditions



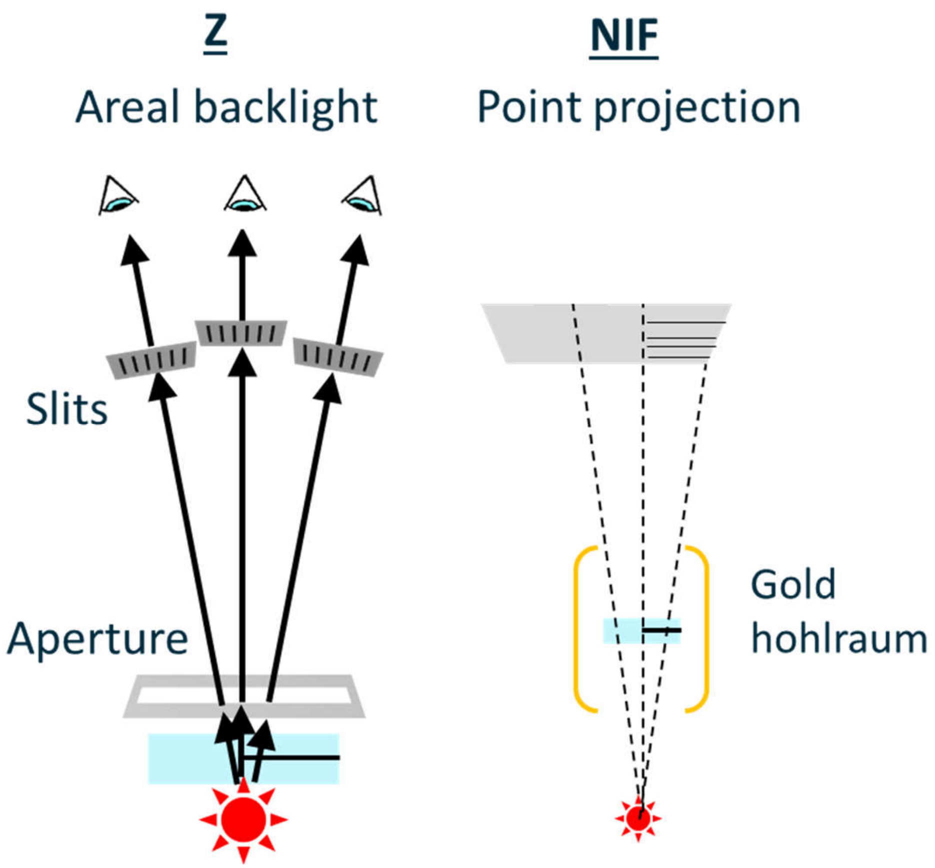
After a refurbishment of the Z machine enabled experiments at higher densities and temperatures, Bailey at al found surprising disagreement between models and experiments

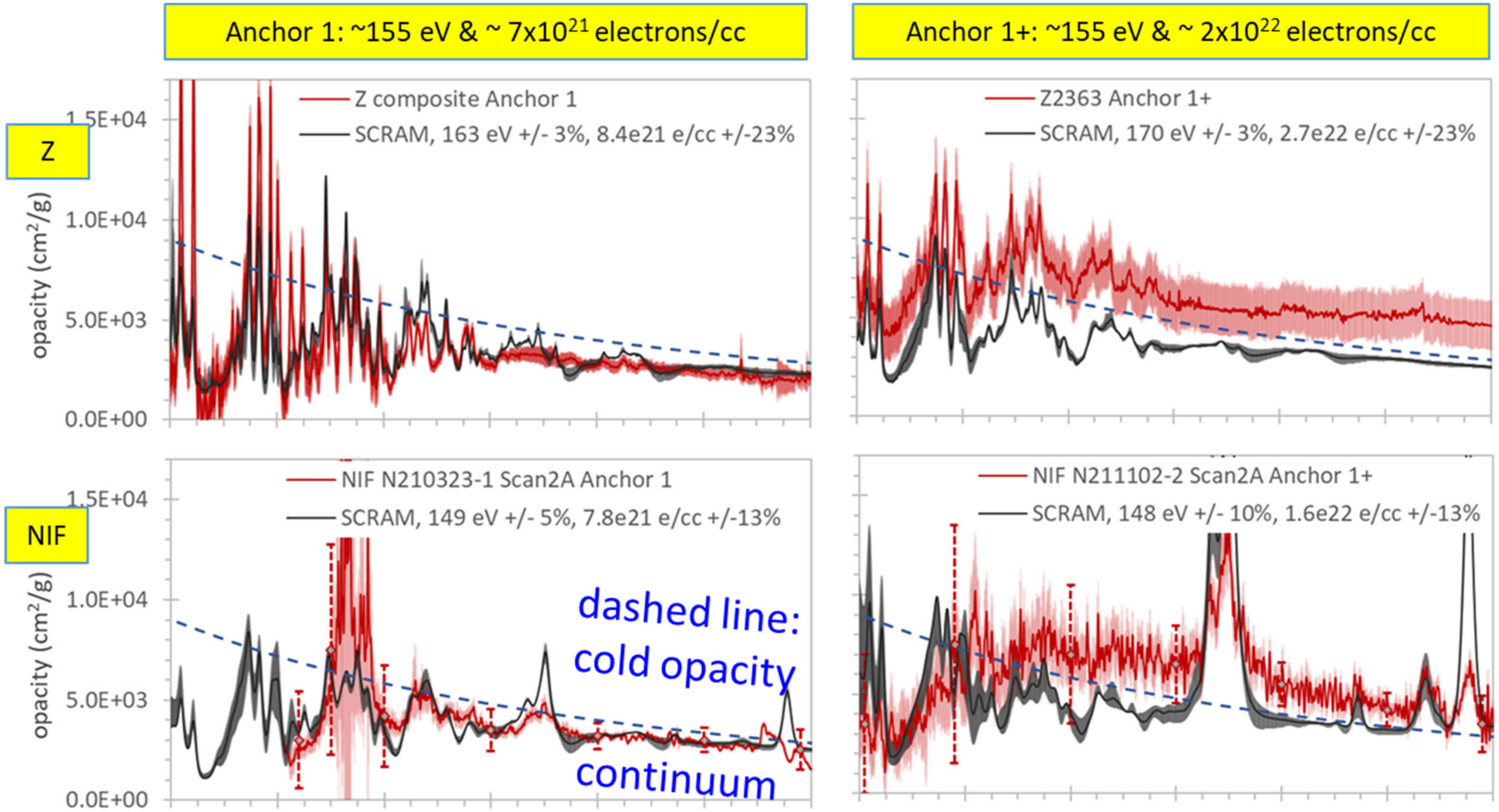


This is one of only a handful of benchmark experiments for high energy density plasmas: we will be surprised again!

Bailey et al, Nature 517, 56 (2015); Nagayama et al PRL 122, 235001 (2019)

The measurements on Z have inspired opacity measurements on NIF, which (so far) show similar results.





Work is ongoing in both experiments and opacity theory!

NIF spectra courtesy Bob Heeter, Ted Perry, Heather Johns et al, diagrams from Tai Nagayama

Conclusions

- Spectroscopy unites the very small – atomic scale & quantum mechanics – with the large (and VERY large!) – laboratory plasmas, fusion, and astrophysics

- X-ray spectroscopy can provide detailed information about HED plasmas beyond yields and imaging, including plasma composition (mix), temperature, density, velocity, and EM fields

- Benchmark-quality experiments to test atomic and spectroscopic models are difficult, requiring careful sample preparation and independent sample characterization,
  -- and they are /critical/ to increasing our understanding of models and calibrating our confidence in plasma simulations

- Mark Herrmann: *If we can measure a thing, we can make it better*
  For ICF experiments on NIF, Z, and Omega, X-ray and neutron spectroscopy have been essential tools to help understand and optimize fusion target performance

Thank you!

Questions?